Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 02:23 AM EDT

PDB ID	:	3ERR
Title	:	Microtubule binding domain from mouse cytoplasmic dynein as a fusion with seryl-tRNA synthetase
Authors	:	Carter, A.P.
Deposited on	:	2008-10-03
Resolution	:	2.27 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:

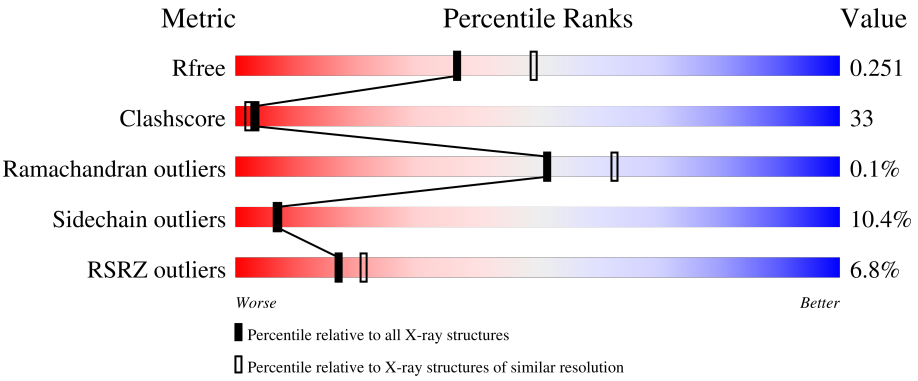
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	536	4% 65% 28% 5%
1	B	536	10% 54% 38% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8589 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 fusion protein of microtubule binding domain from mouse cytoplasmic dynein and seryl-tRNA synthetase from Thermus thermophilus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4210	2677	741	776	16			
1	B	527	Total	C	N	O	S	0	0	0
			4210	2677	741	776	16			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9JHU4
A	2	VAL	-	expression tag	UNP Q9JHU4
A	3	ASP	-	expression tag	UNP Q9JHU4
A	4	LEU	-	expression tag	UNP Q9JHU4
A	5	LYS	-	expression tag	UNP Q9JHU4
A	6	ARG	-	expression tag	UNP Q9JHU4
A	7	LEU	-	expression tag	UNP Q9JHU4
A	8	ARG	-	expression tag	UNP Q9JHU4
A	9	GLN	-	expression tag	UNP Q9JHU4
A	10	GLU	-	expression tag	UNP Q9JHU4
A	11	PRO	-	expression tag	UNP Q9JHU4
A	12	GLU	-	expression tag	UNP Q9JHU4
A	13	VAL	-	expression tag	UNP Q9JHU4
A	14	PHE	-	expression tag	UNP Q9JHU4
A	15	HIS	-	expression tag	UNP Q9JHU4
A	16	ARG	-	expression tag	UNP Q9JHU4
A	17	ALA	-	expression tag	UNP Q9JHU4
A	18	ILE	-	expression tag	UNP Q9JHU4
A	19	ARG	-	expression tag	UNP Q9JHU4
A	20	GLU	-	expression tag	UNP Q9JHU4
A	21	LYS	-	expression tag	UNP Q9JHU4
A	22	GLY	-	expression tag	UNP Q9JHU4
A	23	VAL	-	expression tag	UNP Q9JHU4
A	24	ALA	-	expression tag	UNP Q9JHU4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	LEU	-	expression tag	UNP Q9JHU4
A	26	ASP	-	expression tag	UNP Q9JHU4
A	27	LEU	-	expression tag	UNP Q9JHU4
A	28	GLU	-	expression tag	UNP Q9JHU4
A	29	ALA	-	expression tag	UNP Q9JHU4
A	30	LEU	-	expression tag	UNP Q9JHU4
A	31	LEU	-	expression tag	UNP Q9JHU4
A	32	ALA	-	expression tag	UNP Q9JHU4
A	33	VAL	-	expression tag	UNP Q9JHU4
A	34	ASP	-	expression tag	UNP Q9JHU4
A	3323	ALA	CYS	engineered mutation	UNP Q9JHU4
A	3387	ALA	CYS	engineered mutation	UNP Q9JHU4
A	420	GLY	-	expression tag	UNP P34945
A	421	ALA	-	expression tag	UNP P34945
A	422	HIS	-	expression tag	UNP P34945
A	423	HIS	-	expression tag	UNP P34945
A	424	HIS	-	expression tag	UNP P34945
A	425	HIS	-	expression tag	UNP P34945
A	426	HIS	-	expression tag	UNP P34945
A	427	HIS	-	expression tag	UNP P34945
B	1	MET	-	expression tag	UNP Q9JHU4
B	2	VAL	-	expression tag	UNP Q9JHU4
B	3	ASP	-	expression tag	UNP Q9JHU4
B	4	LEU	-	expression tag	UNP Q9JHU4
B	5	LYS	-	expression tag	UNP Q9JHU4
B	6	ARG	-	expression tag	UNP Q9JHU4
B	7	LEU	-	expression tag	UNP Q9JHU4
B	8	ARG	-	expression tag	UNP Q9JHU4
B	9	GLN	-	expression tag	UNP Q9JHU4
B	10	GLU	-	expression tag	UNP Q9JHU4
B	11	PRO	-	expression tag	UNP Q9JHU4
B	12	GLU	-	expression tag	UNP Q9JHU4
B	13	VAL	-	expression tag	UNP Q9JHU4
B	14	PHE	-	expression tag	UNP Q9JHU4
B	15	HIS	-	expression tag	UNP Q9JHU4
B	16	ARG	-	expression tag	UNP Q9JHU4
B	17	ALA	-	expression tag	UNP Q9JHU4
B	18	ILE	-	expression tag	UNP Q9JHU4
B	19	ARG	-	expression tag	UNP Q9JHU4
B	20	GLU	-	expression tag	UNP Q9JHU4
B	21	LYS	-	expression tag	UNP Q9JHU4
B	22	GLY	-	expression tag	UNP Q9JHU4

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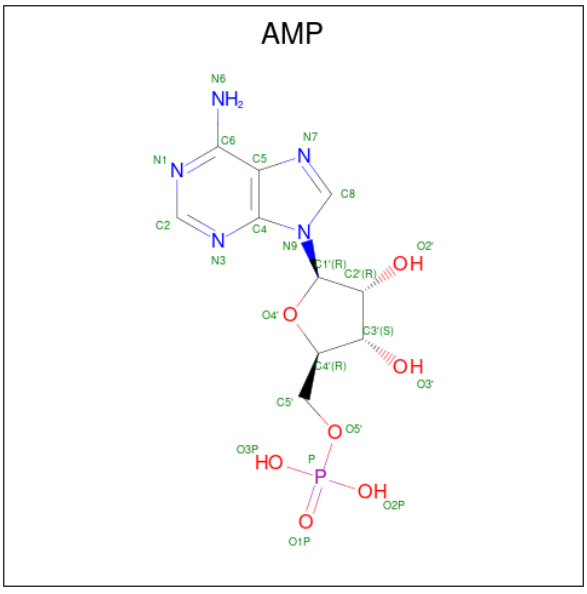
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	VAL	-	expression tag	UNP Q9JHU4
B	24	ALA	-	expression tag	UNP Q9JHU4
B	25	LEU	-	expression tag	UNP Q9JHU4
B	26	ASP	-	expression tag	UNP Q9JHU4
B	27	LEU	-	expression tag	UNP Q9JHU4
B	28	GLU	-	expression tag	UNP Q9JHU4
B	29	ALA	-	expression tag	UNP Q9JHU4
B	30	LEU	-	expression tag	UNP Q9JHU4
B	31	LEU	-	expression tag	UNP Q9JHU4
B	32	ALA	-	expression tag	UNP Q9JHU4
B	33	VAL	-	expression tag	UNP Q9JHU4
B	34	ASP	-	expression tag	UNP Q9JHU4
B	3323	ALA	CYS	engineered mutation	UNP Q9JHU4
B	3387	ALA	CYS	engineered mutation	UNP Q9JHU4
B	420	GLY	-	expression tag	UNP P34945
B	421	ALA	-	expression tag	UNP P34945
B	422	HIS	-	expression tag	UNP P34945
B	423	HIS	-	expression tag	UNP P34945
B	424	HIS	-	expression tag	UNP P34945
B	425	HIS	-	expression tag	UNP P34945
B	426	HIS	-	expression tag	UNP P34945
B	427	HIS	-	expression tag	UNP P34945

- 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		

- Molecule 3 is water.

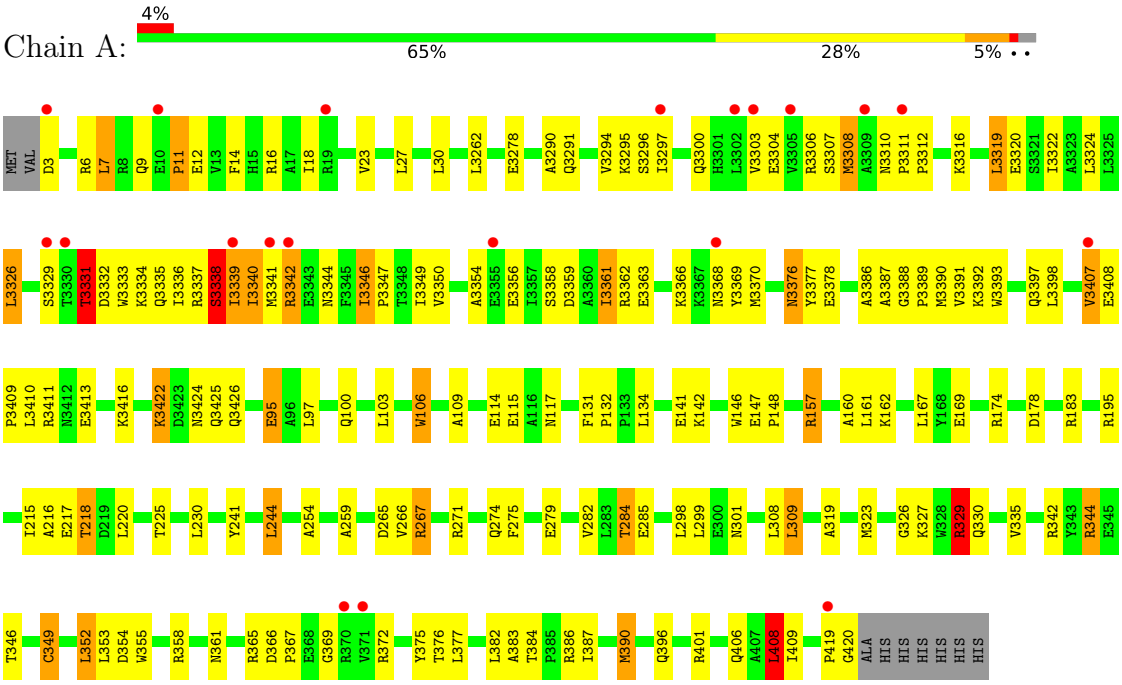
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	52	Total	O	0	0
			52	52		

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.

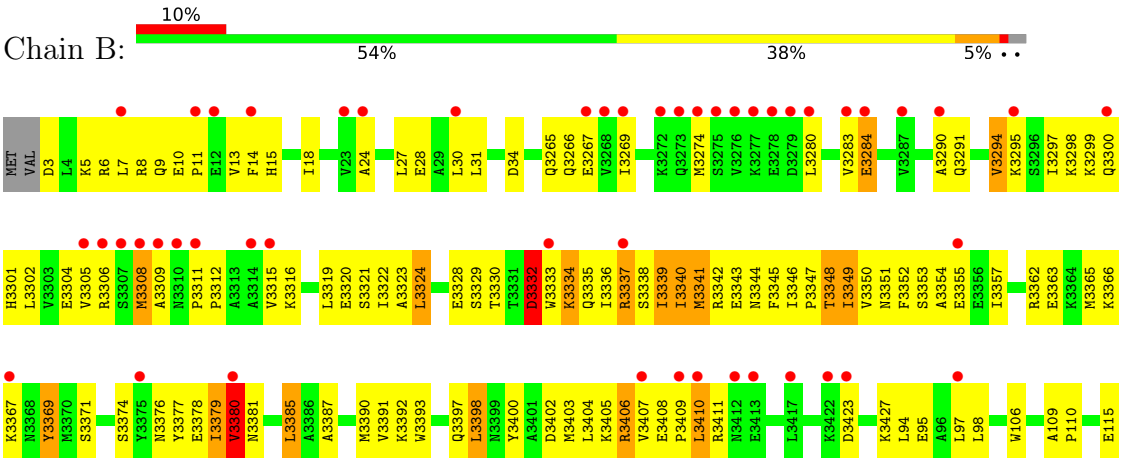
• Molecule 1: fusion protein of microtubule binding domain from mouse cytoplasmic dynein and seryl-tRNA synthetase from Thermus thermophilus

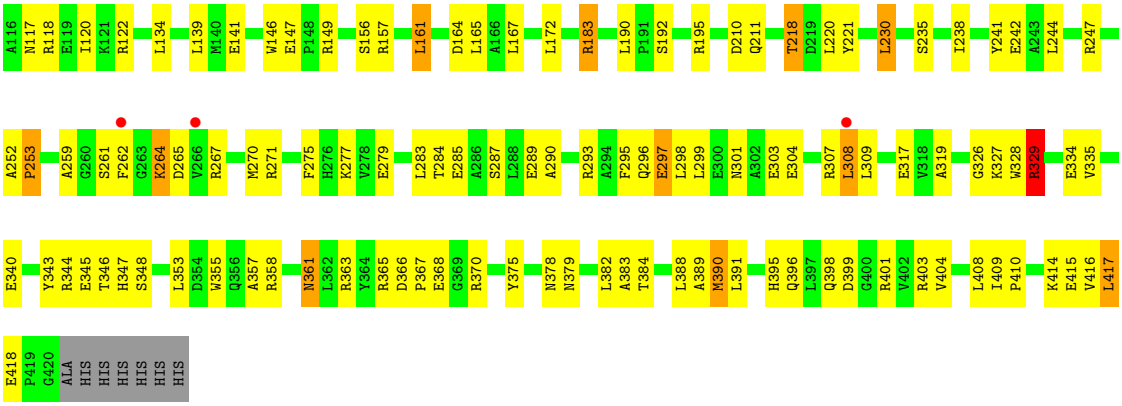
Chain A:



• Molecule 1: fusion protein of microtubule binding domain from mouse cytoplasmic dynein and seryl-tRNA synthetase from Thermus thermophilus

Chain B:




A116 N117 R118 E119 I120 K121 R122 L134 L139 M140 E141 W146 E147 P148 R149 S156 R157 L161 D164 L165 A166 L167 L172 R183 L190 P191 S192 R195 D210 Q211 T218 D219 L220 Y221 L230 S235 I238 Y241 E242 A243 L244 R247
A252 P253 A259 G260 S261 F262 G263 K264 D265 V266 R267 M270 R271 F275 H276 K277 V278 E279 L283 T284 E285 A286 S287 L288 E289 A290 R293 A294 F295 Q296 E297 L298 L299 E300 N301 A302 E303 E304 R307 L308 L309 E317 V318 A319 G326 K327 W328 R329 E334 V335
E340 Y343 R344 E345 T346 H347 S348 L353 D354 W355 Q356 A357 R358 N361 L362 R363 Y364 R365 D366 P367 E368 G369 R370 Y375 N378 N379 L382 A383 T384 L388 A389 M390 L391 H395 Q396 L397 Q398 D399 G400 R401 V402 R403 V404 L408 I409 P410 K414 E415 V416 L417
E418 P419 G420 ALA HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	144.30Å 144.30Å 159.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.27 – 2.27 49.24 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.27-2.27) 99.1 (49.24-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.197 , 0.247 0.220 , 0.251	Depositor DCC
R_{free} test set	2868 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8589	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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	0.99	6/4301 (0.1%)	0.99	16/5828 (0.3%)
1	B	0.90	6/4301 (0.1%)	0.93	14/5828 (0.2%)
All	All	0.95	12/8602 (0.1%)	0.96	30/11656 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	GLY	CA-C	7.26	1.63	1.51
1	A	349	CYS	CB-SG	-6.83	1.70	1.82
1	B	115	GLU	CD-OE2	6.31	1.32	1.25
1	A	115	GLU	CG-CD	6.02	1.60	1.51
1	A	3278	GLU	CB-CG	-5.92	1.40	1.52
1	B	295	PHE	CE2-CZ	5.73	1.48	1.37
1	B	297	GLU	CD-OE2	5.62	1.31	1.25
1	A	169	GLU	CD-OE2	5.61	1.31	1.25
1	B	115	GLU	CD-OE1	5.55	1.31	1.25
1	B	221	TYR	CD1-CE1	5.23	1.47	1.39
1	B	3309	ALA	C-O	5.18	1.33	1.23
1	A	95	GLU	CB-CG	5.15	1.61	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	ARG	NE-CZ-NH1	12.33	126.46	120.30
1	A	344	ARG	NE-CZ-NH1	-12.18	114.21	120.30
1	A	329	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	A	408	LEU	CA-CB-CG	-9.66	93.08	115.30
1	A	344	ARG	NE-CZ-NH2	9.39	124.99	120.30
1	B	329	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	B	253	PRO	CA-N-CD	-8.88	99.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	157	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	B	3380	VAL	CB-CA-C	-8.53	95.19	111.40
1	B	183	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	A	157	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	329	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	408	LEU	CA-CB-CG	-6.91	99.41	115.30
1	B	271	ARG	N-CA-C	-6.86	92.49	111.00
1	A	323	MET	CG-SD-CE	-6.69	89.50	100.20
1	B	122	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	195	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	195	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	3331	THR	CB-CA-C	-5.84	95.83	111.60
1	A	299	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	3338	SER	CB-CA-C	-5.68	99.31	110.10
1	A	352	LEU	CB-CA-C	5.66	120.96	110.20
1	B	3332	ASP	N-CA-C	-5.65	95.75	111.00
1	A	386	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	259	ALA	C-N-CA	-5.59	110.57	122.30
1	B	183	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	403	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	307	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	24	ALA	CB-CA-C	5.08	117.72	110.10
1	B	3369	TYR	CB-CA-C	-5.02	100.35	110.40

There are no chirality outliers.

There are no planarity outliers.

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	4210	0	4230	238	0
1	B	4210	0	4230	323	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
3	A	71	0	0	2	0
3	B	52	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8589	0	8484	558	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (558) 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:B:7:LEU:HD12	1:B:14:PHE:CD2	1.52	1.44
1:B:3308:MET:SD	1:B:3311:PRO:HB3	1.58	1.43
1:A:3339:ILE:HD13	1:A:3340:ILE:N	1.33	1.41
1:A:3308:MET:CE	1:A:3312:PRO:HD2	1.55	1.34
1:B:3340:ILE:HA	1:B:3345:PHE:CD1	1.64	1.32
1:B:7:LEU:HD12	1:B:14:PHE:CE2	1.66	1.28
1:B:3332:ASP:O	1:B:3336:ILE:HD12	1.36	1.21
1:B:3376:ASN:O	1:B:3380:VAL:HG22	1.40	1.19
1:A:3407:VAL:CG1	1:A:3411:ARG:HD2	1.70	1.19
1:B:3294:VAL:HG11	1:B:3349:ILE:HD11	1.24	1.17
1:B:3319:LEU:HD12	1:B:3333:TRP:CH2	1.77	1.16
1:B:3337:ARG:HG3	1:B:3337:ARG:HH11	1.00	1.16
1:B:3344:ASN:O	1:B:3348:THR:HG23	1.45	1.13
1:B:7:LEU:HA	1:B:14:PHE:CE2	1.84	1.12
1:B:10:GLU:HB3	1:B:13:VAL:HG23	1.31	1.12
1:B:3324:LEU:HD12	1:B:3365:MET:HG2	1.30	1.13
1:B:183:ARG:HD2	1:B:301:ASN:ND2	1.63	1.13
1:B:3319:LEU:HD12	1:B:3333:TRP:HH2	0.99	1.12
1:B:3355:GLU:OE2	1:B:3404:LEU:HD13	1.46	1.12
1:B:8:ARG:O	1:B:11:PRO:HD3	1.50	1.12
1:B:3387:ALA:HA	1:B:3390:MET:CE	1.79	1.12
1:B:183:ARG:HD2	1:B:301:ASN:HD21	0.98	1.12
1:B:3337:ARG:HH11	1:B:3337:ARG:CG	1.61	1.11
1:A:3316:LYS:HE3	1:A:3320:GLU:OE2	1.51	1.10
1:A:3346:ILE:HD12	1:A:3346:ILE:N	1.59	1.10
1:A:3361:ILE:C	1:A:3361:ILE:HD12	1.72	1.09
1:A:3346:ILE:HD13	1:A:3347:PRO:HD3	1.22	1.09
1:A:3294:VAL:O	1:A:3297:ILE:HG13	1.50	1.09
1:A:3346:ILE:H	1:A:3346:ILE:CD1	1.63	1.08
1:A:3311:PRO:HG3	1:A:3333:TRP:CZ2	1.87	1.07
1:B:7:LEU:CD1	1:B:14:PHE:CD2	2.40	1.04
1:A:3361:ILE:C	1:A:3361:ILE:CD1	2.27	1.04
1:A:3308:MET:HE1	1:A:3312:PRO:HD2	1.06	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3346:ILE:HD12	1:A:3346:ILE:H	0.87	1.03
1:A:3358:SER:OG	1:A:3361:ILE:HG22	1.57	1.03
1:A:3407:VAL:HG12	1:A:3411:ARG:HD2	1.40	1.01
1:B:3308:MET:SD	1:B:3311:PRO:CB	2.48	1.01
1:B:3340:ILE:HA	1:B:3345:PHE:CE1	1.94	1.01
1:B:3387:ALA:HA	1:B:3390:MET:HE2	1.02	1.01
1:B:3332:ASP:HB3	1:B:3335:GLN:HG3	1.42	1.00
1:A:267:ARG:H	1:A:267:ARG:HD3	1.24	1.00
1:B:110:PRO:HG3	1:B:118:ARG:CZ	1.92	0.99
1:B:3337:ARG:HG3	1:B:3337:ARG:NH1	1.72	0.98
1:A:3308:MET:HE1	1:A:3312:PRO:CD	1.92	0.98
1:A:3322:ILE:HD11	1:A:3390:MET:CB	1.91	0.98
1:A:3322:ILE:CD1	1:A:3390:MET:HB3	1.93	0.98
1:B:3301:HIS:HA	1:B:3304:GLU:HG2	1.42	0.98
1:A:3322:ILE:HD11	1:A:3390:MET:HB3	1.00	0.98
1:B:3423:ASP:O	1:B:3427:LYS:HG2	1.64	0.98
1:B:289:GLU:HG2	1:B:293:ARG:HH12	1.29	0.97
1:A:3308:MET:CE	1:A:3312:PRO:CD	2.42	0.97
1:A:3346:ILE:CD1	1:A:3347:PRO:HD3	1.93	0.97
1:B:3324:LEU:CD1	1:B:3365:MET:HG2	1.93	0.97
1:B:10:GLU:HB3	1:B:13:VAL:CG2	1.95	0.97
1:B:218:THR:HG23	1:B:220:LEU:H	1.28	0.97
1:B:3320:GLU:HG2	1:B:3369:TYR:OH	1.63	0.96
1:A:284:THR:HG22	1:A:375:TYR:HB2	1.45	0.96
1:B:3322:ILE:HD11	1:B:3390:MET:HB3	1.45	0.96
1:B:3387:ALA:CA	1:B:3390:MET:HE2	1.95	0.96
1:A:3339:ILE:HD13	1:A:3339:ILE:C	1.81	0.95
1:B:14:PHE:O	1:B:18:ILE:HG13	1.67	0.95
1:A:3332:ASP:OD1	1:A:3335:GLN:HG3	1.67	0.94
1:B:270:MET:CE	1:B:389:ALA:CB	2.45	0.94
1:B:270:MET:CE	1:B:389:ALA:HB3	1.98	0.93
1:B:7:LEU:CD1	1:B:14:PHE:CG	2.51	0.93
1:A:3386:ALA:O	1:A:3390:MET:HE3	1.68	0.93
1:B:11:PRO:O	1:B:15:HIS:HD2	1.50	0.93
1:B:3316:LYS:HE2	3:B:3479:HOH:O	1.69	0.92
1:A:267:ARG:H	1:A:267:ARG:CD	1.82	0.92
1:A:3339:ILE:CD1	1:A:3340:ILE:N	2.30	0.92
1:A:3346:ILE:HD13	1:A:3347:PRO:CD	2.01	0.91
1:A:3361:ILE:CD1	1:A:3361:ILE:O	2.19	0.91
1:B:270:MET:HE1	1:B:389:ALA:HB3	1.49	0.91
1:B:192:SER:OG	1:B:253:PRO:HD2	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:CD1	1:B:14:PHE:CE2	2.51	0.91
1:A:3:ASP:OD2	1:A:6:ARG:HG3	1.71	0.91
1:A:3339:ILE:HA	1:A:3342:ARG:HG3	1.53	0.90
1:B:289:GLU:CG	1:B:293:ARG:HH12	1.84	0.90
1:B:7:LEU:HD12	1:B:14:PHE:CG	2.06	0.90
1:A:3425:GLN:O	1:A:95:GLU:HG3	1.72	0.89
1:A:267:ARG:CD	1:A:267:ARG:N	2.35	0.89
1:B:218:THR:CG2	1:B:220:LEU:H	1.84	0.89
1:B:289:GLU:HG2	1:B:293:ARG:NH1	1.87	0.89
1:B:3294:VAL:HG11	1:B:3349:ILE:CD1	2.04	0.88
1:B:7:LEU:HA	1:B:14:PHE:HE2	1.34	0.88
1:B:10:GLU:OE1	1:B:13:VAL:HG21	1.72	0.88
1:A:30:LEU:HD13	1:A:97:LEU:HB3	1.55	0.87
1:B:3408:GLU:HB3	1:B:3409:PRO:HD3	1.57	0.87
1:A:3361:ILE:O	1:A:3361:ILE:HD13	1.74	0.87
1:B:3335:GLN:O	1:B:3339:ILE:HG12	1.74	0.87
1:B:3376:ASN:HB3	1:B:3379:ILE:HB	1.56	0.86
1:A:3331:THR:HG23	1:A:3331:THR:O	1.75	0.86
1:A:3316:LYS:CE	1:A:3320:GLU:OE2	2.22	0.86
1:B:3312:PRO:O	1:B:3315:VAL:HG22	1.74	0.86
1:B:3409:PRO:HG2	1:B:3410:LEU:CD2	2.07	0.85
1:A:3339:ILE:HD13	1:A:3340:ILE:H	1.41	0.85
1:B:192:SER:OG	1:B:253:PRO:CD	2.24	0.85
1:B:346:THR:CG2	1:B:390:MET:HE3	2.05	0.85
1:A:3407:VAL:CG1	1:A:3411:ARG:CD	2.55	0.84
1:B:3301:HIS:CA	1:B:3304:GLU:HG2	2.06	0.84
1:B:3319:LEU:CD1	1:B:3333:TRP:HH2	1.88	0.84
1:B:3340:ILE:HA	1:B:3345:PHE:HD1	1.38	0.84
1:B:3406:ARG:O	1:B:3410:LEU:HD23	1.77	0.84
1:B:3340:ILE:CA	1:B:3345:PHE:CD1	2.57	0.83
1:B:11:PRO:O	1:B:15:HIS:CD2	2.32	0.83
1:A:3308:MET:HE2	1:A:3311:PRO:HA	1.61	0.83
1:A:3324:LEU:HD23	1:A:3324:LEU:C	1.97	0.82
1:A:3388:GLY:O	1:A:3391:VAL:HG12	1.79	0.82
1:A:3300:GLN:O	1:A:3303:VAL:HG12	1.79	0.82
1:A:3425:GLN:HG3	1:A:95:GLU:OE1	1.79	0.82
1:A:3311:PRO:HG3	1:A:3333:TRP:CE2	2.14	0.82
1:A:3407:VAL:HG12	1:A:3411:ARG:CD	2.10	0.82
1:B:8:ARG:HE	1:B:31:LEU:HD22	1.45	0.81
1:A:3322:ILE:O	1:A:3326:LEU:HD22	1.80	0.81
1:B:3311:PRO:HB2	1:B:3315:VAL:HG21	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASP:OD2	1:A:6:ARG:CD	2.29	0.81
1:B:6:ARG:HH12	1:B:358:ARG:NH2	1.77	0.81
1:A:3:ASP:OD2	1:A:6:ARG:CG	2.29	0.81
1:B:3291:GLN:O	1:B:3295:LYS:HE3	1.80	0.81
1:A:134:LEU:H	1:A:396:GLN:HE22	1.26	0.80
1:A:382:LEU:HD23	1:A:383:ALA:N	1.97	0.80
1:B:3344:ASN:O	1:B:3348:THR:CG2	2.27	0.80
1:B:3336:ILE:O	1:B:3340:ILE:CG2	2.30	0.80
1:B:3302:LEU:O	1:B:3306:ARG:HG2	1.81	0.80
1:B:8:ARG:O	1:B:11:PRO:CD	2.31	0.79
1:B:192:SER:OG	1:B:253:PRO:HG2	1.83	0.79
1:B:3298:LYS:HB2	1:B:3301:HIS:CE1	2.17	0.78
1:A:30:LEU:HD13	1:A:97:LEU:CB	2.14	0.77
1:B:3363:GLU:O	1:B:3367:LYS:HG3	1.84	0.77
1:B:3316:LYS:HG2	1:B:3333:TRP:CE3	2.20	0.77
1:A:3358:SER:OG	1:A:3361:ILE:CG2	2.32	0.77
1:A:218:THR:CG2	1:A:220:LEU:H	1.98	0.77
1:B:3328:GLU:HG3	1:B:3328:GLU:O	1.83	0.76
1:B:3322:ILE:CD1	1:B:3390:MET:HB3	2.14	0.76
1:B:3407:VAL:CG1	1:B:3411:ARG:CD	2.62	0.76
1:B:106:TRP:NE1	1:B:329:ARG:HG2	2.01	0.76
1:A:3346:ILE:CD1	1:A:3347:PRO:CD	2.62	0.76
1:B:3376:ASN:O	1:B:3380:VAL:CG2	2.29	0.76
1:B:3410:LEU:N	1:B:3410:LEU:HD22	2.00	0.76
1:B:147:GLU:OE2	1:B:149:ARG:HG3	1.84	0.76
1:B:3301:HIS:HA	1:B:3304:GLU:CG	2.16	0.76
1:B:3311:PRO:HB2	1:B:3315:VAL:CG2	2.14	0.76
1:B:3336:ILE:O	1:B:3340:ILE:HG23	1.85	0.76
1:B:7:LEU:HD13	1:B:14:PHE:CE1	2.21	0.76
1:B:3410:LEU:CD2	1:B:3410:LEU:N	2.48	0.76
1:A:3308:MET:CE	1:A:3311:PRO:HA	2.16	0.75
1:B:284:THR:CG2	1:B:290:ALA:HB1	2.16	0.75
1:B:3407:VAL:HG12	1:B:3411:ARG:HD3	1.68	0.75
1:B:117:ASN:ND2	1:B:319:ALA:H	1.84	0.75
1:B:3406:ARG:O	1:B:3410:LEU:CD2	2.33	0.75
1:B:3355:GLU:OE2	1:B:3404:LEU:CD1	2.31	0.75
1:B:7:LEU:CD1	1:B:14:PHE:CD1	2.70	0.75
1:B:3410:LEU:CD2	1:B:3410:LEU:H	2.00	0.75
1:B:3312:PRO:HG2	1:B:3315:VAL:HG13	1.68	0.74
1:B:3407:VAL:HG12	1:B:3411:ARG:CD	2.18	0.74
1:B:3319:LEU:CD1	1:B:3333:TRP:CH2	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:HG2	1:A:372:ARG:HH11	1.53	0.74
1:B:7:LEU:CD1	1:B:14:PHE:CZ	2.71	0.73
1:B:3408:GLU:HB3	1:B:3409:PRO:CD	2.18	0.73
1:B:335:VAL:HG12	1:B:390:MET:HG2	1.69	0.73
1:A:3322:ILE:O	1:A:3326:LEU:CD2	2.38	0.72
1:B:3409:PRO:HG2	1:B:3410:LEU:HD22	1.71	0.72
1:A:11:PRO:HG2	1:A:12:GLU:OE1	1.89	0.72
1:B:317:GLU:OE2	1:B:329:ARG:HD3	1.89	0.72
1:B:3283:VAL:HG11	1:B:3400:TYR:CA	2.18	0.72
1:B:157:ARG:NH1	1:B:265:ASP:O	2.22	0.72
1:B:192:SER:OG	1:B:253:PRO:CG	2.38	0.72
1:B:3316:LYS:HA	1:B:3333:TRP:CZ3	2.25	0.72
1:B:238:ILE:HD11	1:B:363:ARG:NH2	2.05	0.71
1:A:3386:ALA:O	1:A:3390:MET:CE	2.38	0.71
1:B:3306:ARG:HB3	1:B:3340:ILE:HD11	1.71	0.71
1:B:366:ASP:OD2	1:B:370:ARG:HG2	1.90	0.71
1:A:3366:LYS:HE3	1:A:3398:LEU:HD11	1.72	0.71
1:A:3324:LEU:CD2	1:A:3361:ILE:HG12	2.20	0.71
1:B:106:TRP:CD1	1:B:329:ARG:HG2	2.25	0.71
1:B:3407:VAL:CG1	1:B:3411:ARG:HD2	2.19	0.71
1:A:3346:ILE:N	1:A:3346:ILE:CD1	2.35	0.70
1:A:117:ASN:ND2	1:A:319:ALA:H	1.88	0.70
1:A:12:GLU:HB3	1:A:16:ARG:HH12	1.56	0.69
1:A:3311:PRO:CG	1:A:3333:TRP:CE2	2.74	0.69
1:A:372:ARG:HG2	1:A:372:ARG:NH1	2.05	0.69
1:A:12:GLU:HB3	1:A:16:ARG:NH1	2.07	0.69
1:B:218:THR:HG23	1:B:220:LEU:N	2.06	0.69
1:A:267:ARG:HD3	1:A:267:ARG:N	1.93	0.69
1:B:3347:PRO:O	1:B:3351:ASN:ND2	2.26	0.69
1:B:3354:ALA:HA	1:B:3357:ILE:HD12	1.75	0.69
1:B:289:GLU:CG	1:B:293:ARG:NH1	2.50	0.69
1:A:267:ARG:N	1:A:267:ARG:HD2	2.07	0.69
1:B:3295:LYS:HG3	1:B:3350:VAL:HG21	1.75	0.69
1:B:3290:ALA:O	1:B:3294:VAL:HG23	1.92	0.69
1:B:275:PHE:HB2	1:B:384:THR:O	1.94	0.68
1:B:3283:VAL:HG11	1:B:3400:TYR:HA	1.74	0.68
1:A:3361:ILE:HD12	1:A:3361:ILE:O	1.88	0.68
1:A:366:ASP:HB2	1:A:367:PRO:CD	2.23	0.68
1:B:3294:VAL:CG1	1:B:3349:ILE:HD11	2.15	0.68
1:A:3388:GLY:O	1:A:3391:VAL:CG1	2.41	0.68
1:A:3358:SER:HG	1:A:3361:ILE:HG22	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:O	1:A:375:TYR:HA	1.94	0.68
1:B:3306:ARG:CB	1:B:3340:ILE:HD11	2.24	0.67
1:A:346:THR:HG21	1:A:390:MET:HE3	1.75	0.67
1:A:354:ASP:O	1:A:358:ARG:HG3	1.94	0.67
1:B:134:LEU:H	1:B:396:GLN:HE22	1.41	0.67
1:A:218:THR:HG23	1:A:220:LEU:H	1.59	0.67
1:A:157:ARG:NH2	1:A:271:ARG:HD2	2.10	0.67
1:B:3312:PRO:HD2	1:B:3315:VAL:HG21	1.77	0.67
1:A:3407:VAL:O	1:A:3411:ARG:HG3	1.95	0.67
1:A:241:TYR:HB2	1:A:365:ARG:O	1.95	0.67
1:A:335:VAL:HB	1:A:390:MET:HE3	1.77	0.67
1:A:3342:ARG:CG	1:A:3342:ARG:HH11	2.09	0.66
1:B:253:PRO:HD2	1:B:253:PRO:O	1.94	0.66
1:B:5:LYS:O	1:B:9:GLN:HG3	1.96	0.66
1:B:3332:ASP:CB	1:B:3335:GLN:HG3	2.20	0.66
1:B:3407:VAL:HG11	1:B:3411:ARG:HD2	1.78	0.66
1:B:3324:LEU:HD12	1:B:3365:MET:CG	2.16	0.65
1:A:366:ASP:HB2	1:A:367:PRO:HD2	1.77	0.65
1:A:406:GLN:HA	1:A:409:ILE:HD12	1.78	0.65
1:A:3339:ILE:HD13	1:A:3340:ILE:CA	2.23	0.65
1:B:8:ARG:NE	1:B:31:LEU:HD22	2.12	0.65
1:B:3403:MET:HA	1:B:3406:ARG:HD3	1.79	0.65
1:A:3425:GLN:HE21	1:A:95:GLU:CG	2.10	0.65
1:B:94:LEU:O	1:B:98:LEU:CD2	2.44	0.65
1:B:241:TYR:HB2	1:B:365:ARG:O	1.97	0.64
1:A:3407:VAL:HG11	1:A:3411:ARG:HD2	1.75	0.64
1:B:3337:ARG:CG	1:B:3337:ARG:NH1	2.34	0.64
1:A:3306:ARG:HD3	1:A:3341:MET:SD	2.37	0.64
1:B:3334:LYS:O	1:B:3337:ARG:HB3	1.98	0.64
1:B:10:GLU:CD	1:B:13:VAL:HG21	2.18	0.64
1:B:346:THR:HG21	1:B:390:MET:HE3	1.79	0.64
1:B:7:LEU:CD1	1:B:14:PHE:CE1	2.80	0.64
1:A:3408:GLU:HB3	1:A:3409:PRO:HD3	1.80	0.63
1:B:3332:ASP:C	1:B:3336:ILE:HD12	2.18	0.63
1:B:3328:GLU:OE1	1:B:3339:ILE:HG21	1.99	0.63
1:A:183:ARG:HD2	1:A:301:ASN:ND2	2.13	0.63
1:B:3354:ALA:HB3	1:B:3400:TYR:HD2	1.64	0.63
1:A:382:LEU:HD23	1:A:382:LEU:C	2.19	0.63
1:B:3324:LEU:CD1	1:B:3365:MET:CG	2.75	0.63
1:A:215:ILE:HB	1:A:218:THR:HG21	1.81	0.62
1:A:3376:ASN:OD1	1:A:3378:GLU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3311:PRO:CG	1:A:3333:TRP:CZ2	2.77	0.62
1:B:3283:VAL:HG11	1:B:3400:TYR:N	2.14	0.62
1:B:3336:ILE:O	1:B:3340:ILE:HG22	1.98	0.62
1:A:401:ARG:CG	1:A:419:PRO:HG3	2.30	0.62
1:B:3406:ARG:O	1:B:3409:PRO:HD2	2.00	0.62
1:B:94:LEU:O	1:B:98:LEU:HD22	2.00	0.62
1:B:3316:LYS:CE	3:B:3479:HOH:O	2.37	0.61
1:B:30:LEU:HD12	1:B:94:LEU:HD12	1.82	0.61
1:A:3359:ASP:O	1:A:3363:GLU:HG3	2.01	0.61
1:A:284:THR:HG23	1:A:285:GLU:O	2.00	0.61
1:A:3294:VAL:O	1:A:3297:ILE:CG1	2.39	0.61
1:B:7:LEU:HD11	1:B:14:PHE:CG	2.35	0.61
1:B:8:ARG:NH2	1:B:34:ASP:OD2	2.34	0.61
1:B:3385:LEU:HB2	3:B:3477:HOH:O	2.00	0.61
1:A:266:VAL:HG22	1:A:267:ARG:HH11	1.66	0.61
1:B:347:HIS:HB3	1:B:379:ASN:HD21	1.65	0.61
1:B:3410:LEU:HD23	1:B:3410:LEU:H	1.64	0.60
1:B:7:LEU:HD13	1:B:14:PHE:CZ	2.34	0.60
1:B:3295:LYS:HG3	1:B:3350:VAL:CG2	2.31	0.60
1:A:7:LEU:HD12	1:A:14:PHE:CE2	2.37	0.60
1:A:3340:ILE:HG22	1:A:3341:MET:HG3	1.83	0.60
1:B:3333:TRP:O	1:B:3337:ARG:HB2	2.00	0.60
1:A:282:VAL:CG2	1:A:298:LEU:HD11	2.32	0.60
1:A:335:VAL:HG12	1:A:390:MET:HG2	1.85	0.59
1:B:270:MET:HE1	1:B:389:ALA:CB	2.18	0.59
1:B:30:LEU:CD1	1:B:94:LEU:HD12	2.33	0.58
1:A:183:ARG:HD2	1:A:301:ASN:HD21	1.68	0.58
1:B:3328:GLU:CD	1:B:3339:ILE:HG21	2.23	0.58
1:B:3312:PRO:HG2	1:B:3315:VAL:CG1	2.31	0.58
1:B:3355:GLU:CD	1:B:3404:LEU:HD13	2.22	0.58
1:B:284:THR:HG21	1:B:290:ALA:HB1	1.85	0.58
1:A:419:PRO:O	1:A:420:GLY:C	2.42	0.58
1:A:3308:MET:HE3	1:A:3312:PRO:HD2	1.74	0.58
1:A:3334:LYS:HA	1:A:3337:ARG:HD3	1.86	0.57
1:A:3425:GLN:HE21	1:A:95:GLU:CD	2.08	0.57
1:A:218:THR:HG22	1:A:220:LEU:H	1.69	0.57
1:A:387:ILE:HD12	1:A:390:MET:HE1	1.87	0.57
1:A:18:ILE:HG23	1:A:23:VAL:O	2.04	0.57
1:A:3316:LYS:NZ	1:A:3320:GLU:OE2	2.38	0.57
1:B:6:ARG:NH1	1:B:358:ARG:NH2	2.51	0.57
1:B:3299:LYS:HA	1:B:3302:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3316:LYS:HA	1:B:3333:TRP:HZ3	1.67	0.57
1:A:3407:VAL:HG13	1:A:3411:ARG:HG3	1.85	0.57
1:B:8:ARG:HE	1:B:31:LEU:CD2	2.15	0.57
1:B:366:ASP:HB2	1:B:367:PRO:CD	2.34	0.57
1:A:3291:GLN:O	1:A:3295:LYS:HG3	2.05	0.57
1:A:106:TRP:CD1	1:A:329:ARG:HG2	2.39	0.57
1:B:3321:SER:O	1:B:3324:LEU:HB3	2.06	0.56
1:A:346:THR:CG2	1:A:390:MET:HE3	2.34	0.56
1:B:3306:ARG:HH11	1:B:3341:MET:HE3	1.69	0.56
1:A:218:THR:HG23	1:A:220:LEU:N	2.19	0.56
1:B:147:GLU:OE2	1:B:149:ARG:CG	2.52	0.56
1:B:3403:MET:HA	1:B:3406:ARG:CD	2.35	0.56
1:A:3324:LEU:HD21	1:A:3361:ILE:HG12	1.87	0.56
1:B:183:ARG:HH11	1:B:301:ASN:ND2	2.03	0.56
1:B:285:GLU:HG3	1:B:287:SER:HB3	1.87	0.56
1:B:3377:TYR:CE1	1:B:3381:ASN:HB2	2.40	0.56
1:A:3344:ASN:C	1:A:3347:PRO:HD2	2.26	0.56
1:A:3407:VAL:HG13	1:A:3411:ARG:HD2	1.81	0.56
1:B:3334:LYS:O	1:B:3338:SER:N	2.30	0.56
1:A:12:GLU:OE1	1:A:12:GLU:N	2.31	0.56
1:A:3342:ARG:HG3	1:A:3342:ARG:NH1	2.21	0.56
1:B:391:LEU:O	1:B:395:HIS:HB2	2.06	0.56
1:B:353:LEU:O	1:B:375:TYR:HA	2.06	0.55
1:A:103:LEU:HD22	1:A:352:LEU:O	2.07	0.55
1:B:7:LEU:CA	1:B:14:PHE:CE2	2.74	0.55
1:B:3283:VAL:O	1:B:3283:VAL:HG12	2.07	0.55
1:B:190:LEU:HD11	1:B:230:LEU:HD13	1.89	0.55
1:A:3422:LYS:O	1:A:3426:GLN:HG3	2.06	0.55
1:A:346:THR:HG21	1:A:390:MET:CE	2.36	0.55
1:A:387:ILE:HD12	1:A:390:MET:CE	2.37	0.55
1:B:3387:ALA:CA	1:B:3390:MET:CE	2.66	0.55
1:B:164:ASP:OD2	1:B:418:GLU:HB2	2.07	0.55
1:A:3308:MET:HE3	1:A:3312:PRO:CD	2.32	0.54
1:B:3291:GLN:C	1:B:3295:LYS:HE3	2.27	0.54
1:B:3323:ALA:HB1	1:B:3328:GLU:O	2.07	0.54
1:B:382:LEU:HD23	1:B:383:ALA:N	2.22	0.54
1:B:7:LEU:HD12	1:B:14:PHE:CZ	2.25	0.54
1:B:3340:ILE:CA	1:B:3345:PHE:CE1	2.81	0.54
1:A:7:LEU:HD12	1:A:14:PHE:CD2	2.43	0.54
1:B:3332:ASP:O	1:B:3336:ILE:CD1	2.31	0.54
1:A:3322:ILE:HD13	1:A:3390:MET:SD	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH1	3:A:3455:HOH:O	2.39	0.54
1:A:216:ALA:O	1:A:217:GLU:HB2	2.07	0.54
1:A:282:VAL:HG23	1:A:298:LEU:HD11	1.90	0.54
1:B:3280:LEU:O	1:B:3284:GLU:HB2	2.07	0.54
1:B:366:ASP:HB2	1:B:367:PRO:HD2	1.88	0.54
1:A:3336:ILE:O	1:A:3339:ILE:HD12	2.08	0.54
1:B:3366:LYS:NZ	1:B:3402:ASP:OD2	2.41	0.54
1:B:3301:HIS:C	1:B:3304:GLU:HG2	2.28	0.54
1:B:382:LEU:HD23	1:B:382:LEU:C	2.28	0.54
1:A:3:ASP:OD2	1:A:6:ARG:HD2	2.08	0.54
1:B:3336:ILE:HA	1:B:3339:ILE:HG13	1.89	0.54
1:A:3342:ARG:CG	1:A:3342:ARG:NH1	2.68	0.53
1:A:141:GLU:O	1:A:142:LYS:C	2.47	0.53
1:A:275:PHE:HB2	1:A:384:THR:O	2.08	0.53
1:A:3407:VAL:HG13	1:A:3411:ARG:CG	2.38	0.53
1:B:3311:PRO:HB2	1:B:3312:PRO:HD2	1.91	0.53
1:B:264:LYS:O	1:B:265:ASP:C	2.46	0.53
1:A:3324:LEU:HD21	1:A:3361:ILE:CG1	2.39	0.53
1:A:3340:ILE:CG2	1:A:3341:MET:HG3	2.38	0.53
1:B:7:LEU:HD13	1:B:14:PHE:CD1	2.43	0.53
1:A:3359:ASP:HA	1:A:3362:ARG:HH11	1.73	0.53
1:A:157:ARG:HH21	1:A:271:ARG:HB3	1.73	0.53
1:B:120:ILE:HD13	1:B:317:GLU:HG2	1.91	0.53
1:B:404:VAL:CG2	1:B:417:LEU:HD13	2.39	0.53
1:A:3316:LYS:O	1:A:3320:GLU:HG3	2.08	0.53
1:B:7:LEU:HA	1:B:14:PHE:CZ	2.42	0.53
1:B:283:LEU:C	1:B:283:LEU:HD23	2.29	0.53
1:B:414:LYS:NZ	1:B:418:GLU:OE1	2.42	0.53
1:A:3332:ASP:CG	1:A:3335:GLN:HG3	2.29	0.52
1:A:3295:LYS:HE2	1:A:3350:VAL:HG22	1.92	0.52
1:A:3324:LEU:HD23	1:A:3361:ILE:HG12	1.91	0.52
1:B:3366:LYS:HE3	1:B:3398:LEU:HD21	1.90	0.52
1:A:3359:ASP:HB3	1:A:3362:ARG:NH1	2.24	0.52
1:B:3:ASP:O	1:B:7:LEU:HB2	2.09	0.52
1:B:3265:GLN:O	1:B:3269:ILE:HG13	2.10	0.52
1:B:270:MET:HE3	1:B:389:ALA:CB	2.38	0.52
1:A:3376:ASN:OD1	1:A:3376:ASN:C	2.48	0.52
1:B:28:GLU:OE1	1:B:28:GLU:N	2.43	0.52
1:A:218:THR:CG2	1:A:220:LEU:HB2	2.40	0.52
1:B:10:GLU:N	1:B:11:PRO:HD3	2.24	0.52
1:B:3376:ASN:O	1:B:3379:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3405:LYS:O	1:B:3408:GLU:HB2	2.10	0.52
1:A:3346:ILE:N	1:A:3347:PRO:CD	2.73	0.52
1:A:309:LEU:HD12	1:A:408:LEU:HD13	1.91	0.52
1:B:3408:GLU:CB	1:B:3409:PRO:CD	2.86	0.52
1:A:266:VAL:H	1:A:267:ARG:NH1	2.08	0.52
1:A:401:ARG:HG3	1:A:419:PRO:HG3	1.92	0.52
1:B:3319:LEU:CD2	1:B:3390:MET:HE3	2.40	0.52
1:B:3403:MET:O	1:B:3406:ARG:HD3	2.10	0.52
1:B:94:LEU:CD1	1:B:98:LEU:HD21	2.40	0.52
1:B:110:PRO:HG3	1:B:118:ARG:NH2	2.25	0.51
1:A:106:TRP:NE1	1:A:329:ARG:HG2	2.25	0.51
1:B:3334:LYS:O	1:B:3337:ARG:CB	2.58	0.51
1:B:3408:GLU:N	1:B:3409:PRO:HD2	2.26	0.51
1:A:27:LEU:HD12	1:A:30:LEU:HD23	1.92	0.51
1:B:3354:ALA:HB3	1:B:3400:TYR:CD2	2.45	0.51
1:A:3324:LEU:C	1:A:3324:LEU:CD2	2.74	0.50
1:A:372:ARG:HH11	1:A:372:ARG:CG	2.22	0.50
1:B:3291:GLN:O	1:B:3295:LYS:CE	2.56	0.50
1:B:3374:SER:O	1:B:3379:ILE:HG21	2.11	0.50
1:B:15:HIS:CD2	1:B:27:LEU:HD23	2.46	0.50
1:B:3298:LYS:HD2	1:B:3301:HIS:CE1	2.47	0.50
1:B:3301:HIS:O	1:B:3304:GLU:HG3	2.12	0.50
1:B:3380:VAL:HG21	1:B:3391:VAL:HG11	1.94	0.50
1:B:195:ARG:HG2	1:B:220:LEU:HD23	1.92	0.50
1:B:277:LYS:NZ	1:B:279:GLU:OE2	2.44	0.50
1:A:3344:ASN:HA	1:A:3347:PRO:HG2	1.93	0.50
1:A:3370:MET:HG3	1:A:3398:LEU:HD21	1.93	0.50
1:B:3377:TYR:CD1	1:B:3381:ASN:HB2	2.46	0.50
1:A:366:ASP:CB	1:A:367:PRO:CD	2.88	0.50
1:A:3:ASP:OD2	1:A:6:ARG:NE	2.45	0.50
1:A:3354:ALA:HB2	1:A:3397:GLN:OE1	2.12	0.50
1:B:3:ASP:OD2	1:B:6:ARG:HB2	2.12	0.50
1:B:3400:TYR:O	1:B:3404:LEU:HG	2.12	0.50
1:B:95:GLU:HA	1:B:98:LEU:HD23	1.93	0.50
1:A:419:PRO:O	1:A:420:GLY:O	2.30	0.50
1:A:131:PHE:HB2	1:A:132:PRO:HD2	1.94	0.49
1:A:215:ILE:O	1:A:218:THR:HG22	2.11	0.49
1:B:30:LEU:HD12	1:B:94:LEU:CD1	2.41	0.49
1:B:3336:ILE:O	1:B:3337:ARG:C	2.47	0.49
1:A:254:ALA:O	1:A:274:GLN:HA	2.12	0.49
1:B:296:GLN:HG2	3:B:3440:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ALA:O	1:B:361:ASN:N	2.47	0.48
1:A:3336:ILE:C	1:A:3338:SER:H	2.16	0.48
1:A:3361:ILE:HD12	1:A:3362:ARG:N	2.26	0.48
1:A:174:ARG:NE	1:A:178:ASP:OD1	2.40	0.48
1:B:3:ASP:OD2	1:B:6:ARG:CB	2.61	0.48
1:B:3407:VAL:HG13	1:B:3411:ARG:HG3	1.94	0.48
1:B:3376:ASN:ND2	1:B:3378:GLU:OE1	2.47	0.48
1:A:3324:LEU:HD23	1:A:3324:LEU:O	2.12	0.48
1:A:3391:VAL:HG13	1:A:3392:LYS:N	2.29	0.48
1:A:3311:PRO:HB2	1:A:3316:LYS:HB2	1.94	0.48
1:A:266:VAL:H	1:A:267:ARG:HH11	1.61	0.48
1:A:3339:ILE:HA	1:A:3342:ARG:NH1	2.28	0.47
1:A:218:THR:HG21	1:A:220:LEU:HB2	1.96	0.47
1:B:3304:GLU:HG3	1:B:3305:VAL:N	2.29	0.47
1:B:3:ASP:HB3	1:B:6:ARG:HB3	1.96	0.47
1:B:94:LEU:O	1:B:98:LEU:HD23	2.14	0.47
1:B:10:GLU:CB	1:B:13:VAL:CG2	2.83	0.47
1:B:3299:LYS:HD2	1:B:3299:LYS:N	2.30	0.47
1:B:192:SER:HG	1:B:253:PRO:HD2	1.76	0.47
1:A:3387:ALA:HA	1:A:3390:MET:HE3	1.97	0.47
1:B:110:PRO:HG3	1:B:118:ARG:NH1	2.27	0.47
1:A:3361:ILE:C	1:A:3361:ILE:HD13	2.17	0.47
1:A:3324:LEU:HD21	1:A:3361:ILE:CD1	2.45	0.47
1:A:376:THR:C	1:A:377:LEU:HD12	2.34	0.47
1:B:3306:ARG:NH1	1:B:3341:MET:HE3	2.29	0.47
1:B:304:GLU:HG3	1:B:308:LEU:HD22	1.97	0.47
1:B:14:PHE:O	1:B:18:ILE:CG1	2.51	0.47
1:B:3406:ARG:O	1:B:3410:LEU:HD21	2.14	0.47
1:B:253:PRO:CD	1:B:253:PRO:O	2.61	0.47
1:A:11:PRO:HG2	1:A:12:GLU:CD	2.36	0.47
1:A:106:TRP:CD1	1:A:109:ALA:HB2	2.49	0.47
1:A:377:LEU:HD12	1:A:377:LEU:N	2.30	0.47
1:B:3335:GLN:O	1:B:3339:ILE:CG1	2.54	0.47
1:B:3405:LYS:O	1:B:3408:GLU:CB	2.63	0.47
1:A:3300:GLN:C	1:A:3303:VAL:HG12	2.35	0.46
1:B:3297:ILE:HG22	1:B:3298:LYS:O	2.15	0.46
1:A:3324:LEU:HD21	1:A:3361:ILE:HD13	1.96	0.46
1:A:335:VAL:HB	1:A:390:MET:CE	2.45	0.46
1:B:157:ARG:HH21	1:B:262:PHE:HA	1.80	0.46
1:B:270:MET:HE2	1:B:389:ALA:CB	2.40	0.46
1:A:3290:ALA:HB1	1:A:3393:TRP:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASN:HD21	1:A:319:ALA:H	1.63	0.46
1:B:3346:ILE:N	1:B:3347:PRO:CD	2.79	0.46
1:B:3333:TRP:O	1:B:3337:ARG:N	2.30	0.46
1:B:3337:ARG:HH11	1:B:3337:ARG:HG2	1.68	0.46
1:B:94:LEU:HD11	1:B:98:LEU:HD21	1.97	0.46
1:A:346:THR:CG2	1:A:390:MET:CE	2.94	0.46
1:B:3362:ARG:NH2	1:B:3405:LYS:HD2	2.31	0.46
1:B:409:ILE:HD13	1:B:415:GLU:HG2	1.98	0.46
1:B:3324:LEU:HA	1:B:3329:SER:HB3	1.98	0.46
1:B:3298:LYS:HB2	1:B:3301:HIS:ND1	2.31	0.45
1:A:11:PRO:CG	1:A:12:GLU:OE1	2.63	0.45
1:B:3328:GLU:O	1:B:3328:GLU:CG	2.54	0.45
1:A:330:GLN:HA	1:A:349:CYS:O	2.16	0.45
1:B:30:LEU:CD1	1:B:94:LEU:CD1	2.95	0.45
1:B:3335:GLN:O	1:B:3338:SER:HB2	2.16	0.45
1:B:3393:TRP:HE1	1:B:3397:GLN:HE21	1.63	0.45
1:B:409:ILE:N	1:B:410:PRO:CD	2.79	0.45
1:A:3368:ASN:HB2	1:A:3369:TYR:CD2	2.52	0.45
1:A:157:ARG:HH21	1:A:271:ARG:HD2	1.82	0.45
1:B:3407:VAL:HG12	1:B:3407:VAL:O	2.16	0.45
1:B:134:LEU:HB2	1:B:139:LEU:HG	1.98	0.45
1:A:30:LEU:CD1	1:A:97:LEU:CB	2.91	0.45
1:B:3330:THR:HG21	1:B:3335:GLN:OE1	2.16	0.45
1:B:3406:ARG:C	1:B:3408:GLU:H	2.20	0.45
1:A:3336:ILE:C	1:A:3338:SER:N	2.68	0.45
1:A:30:LEU:CD1	1:A:97:LEU:HB2	2.47	0.45
1:A:3376:ASN:OD1	1:A:3377:TYR:N	2.50	0.45
1:A:241:TYR:HA	1:A:244:LEU:HD22	1.99	0.45
1:A:401:ARG:HG2	1:A:419:PRO:HG3	1.97	0.45
1:B:3335:GLN:HA	1:B:3338:SER:HB2	1.99	0.45
1:B:270:MET:CE	1:B:389:ALA:HB1	2.38	0.45
1:B:326:GLY:HA3	1:B:355:TRP:CD2	2.52	0.45
1:B:156:SER:O	1:B:157:ARG:HB2	2.17	0.45
1:A:3308:MET:HE2	1:A:3311:PRO:CA	2.38	0.45
1:A:3359:ASP:HB3	1:A:3362:ARG:HH12	1.82	0.45
1:A:274:GLN:HE22	1:B:253:PRO:CG	2.30	0.45
1:B:3319:LEU:HD23	1:B:3390:MET:HE3	1.98	0.45
1:A:3310:ASN:N	1:A:3311:PRO:HD3	2.32	0.44
1:A:3332:ASP:HB3	1:A:3335:GLN:HB2	1.99	0.44
1:A:3346:ILE:HD12	1:A:3347:PRO:CD	2.47	0.44
1:B:3352:PHE:HZ	1:B:3357:ILE:HG13	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASP:O	1:B:7:LEU:CB	2.65	0.44
1:A:160:ALA:HB1	1:B:190:LEU:HD23	2.00	0.44
1:B:3290:ALA:HB1	1:B:3393:TRP:HA	1.99	0.44
1:A:3290:ALA:CB	1:A:3393:TRP:HA	2.48	0.44
1:B:3267:GLU:OE1	1:B:3267:GLU:HA	2.16	0.44
1:B:3306:ARG:NH1	1:B:3341:MET:HA	2.32	0.44
1:A:97:LEU:O	1:A:100:GLN:HB2	2.18	0.44
1:B:8:ARG:O	1:B:11:PRO:CG	2.66	0.44
1:B:211:GLN:OE1	1:B:259:ALA:O	2.34	0.44
1:B:299:LEU:O	1:B:303:GLU:HG3	2.18	0.44
1:B:3301:HIS:HA	1:B:3304:GLU:CD	2.37	0.44
1:B:3378:GLU:H	1:B:3378:GLU:CD	2.21	0.44
1:B:3301:HIS:O	1:B:3304:GLU:CG	2.66	0.43
1:A:3311:PRO:HG3	1:A:3333:TRP:CH2	2.46	0.43
1:A:3311:PRO:HG2	1:A:3333:TRP:CD2	2.52	0.43
1:B:284:THR:HG22	1:B:285:GLU:N	2.33	0.43
1:A:309:LEU:CD1	1:A:408:LEU:HD13	2.48	0.43
1:A:3324:LEU:CD2	1:A:3361:ILE:CG1	2.93	0.43
1:B:192:SER:HG	1:B:253:PRO:CD	2.26	0.43
1:B:247:ARG:HH11	1:B:247:ARG:HD2	1.69	0.43
1:A:3319:LEU:HD13	1:A:3319:LEU:HA	1.61	0.43
1:B:3308:MET:SD	1:B:3311:PRO:CA	3.06	0.43
1:B:3319:LEU:HD21	1:B:3390:MET:CE	2.49	0.43
1:A:7:LEU:HG	1:A:27:LEU:HD11	2.01	0.42
1:A:284:THR:CG2	1:A:285:GLU:O	2.66	0.42
1:A:3413:GLU:HA	1:A:3416:LYS:HD2	2.01	0.42
1:B:345:GLU:HG2	1:B:346:THR:N	2.33	0.42
1:A:3358:SER:O	1:A:3362:ARG:HB2	2.19	0.42
1:B:3339:ILE:HG12	1:B:3339:ILE:H	1.49	0.42
1:B:340:GLU:OE1	1:B:344:ARG:HD3	2.18	0.42
1:A:3334:LYS:O	1:A:3337:ARG:HG2	2.19	0.42
1:A:3392:LYS:NZ	3:A:3479:HOH:O	2.52	0.42
1:A:274:GLN:HE22	1:B:253:PRO:HG2	1.85	0.42
1:A:3324:LEU:CD2	1:A:3361:ILE:CD1	2.97	0.42
1:B:238:ILE:CD1	1:B:363:ARG:NH2	2.79	0.42
1:A:7:LEU:HD12	1:A:7:LEU:HA	1.82	0.42
1:B:3407:VAL:CG1	1:B:3407:VAL:O	2.67	0.42
1:B:172:LEU:HD12	1:B:388:LEU:HD21	2.02	0.42
1:A:3322:ILE:O	1:A:3326:LEU:HD23	2.16	0.41
1:A:147:GLU:HA	1:A:148:PRO:HD2	1.76	0.41
1:B:378:ASN:ND2	3:B:3473:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LEU:CD1	1:B:230:LEU:HD13	2.50	0.41
1:A:3377:TYR:HD1	1:A:3388:GLY:O	2.03	0.41
1:B:30:LEU:HD11	1:B:98:LEU:HD22	2.02	0.41
1:B:261:SER:O	1:B:261:SER:OG	2.12	0.41
1:A:326:GLY:HA3	1:A:355:TRP:CE3	2.56	0.41
1:B:30:LEU:HD13	1:B:97:LEU:HB2	2.03	0.41
1:A:3262:LEU:HD13	1:A:3424:ASN:HB3	2.03	0.41
1:A:3346:ILE:N	1:A:3347:PRO:HD2	2.35	0.41
1:B:3340:ILE:HB	1:B:3345:PHE:CE1	2.54	0.41
1:B:8:ARG:HG2	1:B:31:LEU:HD22	2.01	0.41
1:B:10:GLU:HB3	1:B:13:VAL:HG21	1.94	0.41
1:A:3359:ASP:CB	1:A:3362:ARG:NH1	2.84	0.41
1:B:301:ASN:HD22	1:B:301:ASN:HA	1.65	0.41
1:A:3346:ILE:HD12	1:A:3347:PRO:HD2	2.03	0.41
1:B:3346:ILE:N	1:B:3347:PRO:HD2	2.35	0.41
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.82	0.41
1:B:183:ARG:NH1	1:B:301:ASN:HD22	2.18	0.41
1:B:334:GLU:CB	1:B:343:TYR:HB3	2.51	0.41
1:B:3342:ARG:O	1:B:3343:GLU:C	2.57	0.41
1:A:3290:ALA:HB1	1:A:3393:TRP:CA	2.51	0.40
1:A:3359:ASP:OD1	1:A:3362:ARG:NH1	2.54	0.40
1:A:162:LYS:HB3	1:A:162:LYS:HE2	1.88	0.40
1:A:3297:ILE:HG13	1:A:3297:ILE:H	1.70	0.40
1:B:328:TRP:CE3	1:B:353:LEU:HD11	2.56	0.40
1:A:241:TYR:O	1:A:244:LEU:HB2	2.22	0.40
1:B:3328:GLU:OE2	1:B:3339:ILE:HG21	2.21	0.40
1:B:106:TRP:CD1	1:B:109:ALA:HB2	2.56	0.40
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.91	0.40
1:B:252:ALA:HB1	1:B:253:PRO:CD	2.50	0.40
1:A:265:ASP:OD2	1:A:344:ARG:NH2	2.54	0.40
1:B:3311:PRO:CB	1:B:3312:PRO:HD2	2.51	0.40
1:B:401:ARG:HG3	1:B:416:VAL:HG11	2.02	0.40
1:A:335:VAL:CG1	1:A:390:MET:HG2	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	525/536 (98%)	512 (98%)	12 (2%)	1 (0%)	47 57
1	B	525/536 (98%)	513 (98%)	12 (2%)	0	100 100
All	All	1050/1072 (98%)	1025 (98%)	24 (2%)	1 (0%)	51 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	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	443/451 (98%)	400 (90%)	43 (10%)	8 8
1	B	443/451 (98%)	394 (89%)	49 (11%)	6 6
All	All	886/902 (98%)	794 (90%)	92 (10%)	7 7

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	GLN
1	A	3296	SER
1	A	3304	GLU
1	A	3307	SER

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Mol	Chain	Res	Type
1	A	3308	MET
1	A	3319	LEU
1	A	3326	LEU
1	A	3329	SER
1	A	3331	THR
1	A	3338	SER
1	A	3339	ILE
1	A	3340	ILE
1	A	3342	ARG
1	A	3346	ILE
1	A	3349	ILE
1	A	3356	GLU
1	A	3361	ILE
1	A	3376	ASN
1	A	3389	PRO
1	A	3407	VAL
1	A	3410	LEU
1	A	3422	LYS
1	A	106	TRP
1	A	114	GLU
1	A	146	TRP
1	A	161	LEU
1	A	167	LEU
1	A	218	THR
1	A	225	THR
1	A	230	LEU
1	A	244	LEU
1	A	267	ARG
1	A	279	GLU
1	A	284	THR
1	A	308	LEU
1	A	309	LEU
1	A	327	LYS
1	A	329	ARG
1	A	342	ARG
1	A	361	ASN
1	A	390	MET
1	A	408	LEU
1	B	3266	GLN
1	B	3274	MET
1	B	3284	GLU
1	B	3294	VAL

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Mol	Chain	Res	Type
1	B	3300	GLN
1	B	3308	MET
1	B	3324	LEU
1	B	3332	ASP
1	B	3334	LYS
1	B	3337	ARG
1	B	3339	ILE
1	B	3340	ILE
1	B	3341	MET
1	B	3348	THR
1	B	3349	ILE
1	B	3353	SER
1	B	3371	SER
1	B	3379	ILE
1	B	3380	VAL
1	B	3385	LEU
1	B	3392	LYS
1	B	3398	LEU
1	B	3406	ARG
1	B	3410	LEU
1	B	141	GLU
1	B	146	TRP
1	B	161	LEU
1	B	167	LEU
1	B	210	ASP
1	B	218	THR
1	B	230	LEU
1	B	235	SER
1	B	242	GLU
1	B	244	LEU
1	B	264	LYS
1	B	267	ARG
1	B	297	GLU
1	B	298	LEU
1	B	308	LEU
1	B	309	LEU
1	B	327	LYS
1	B	329	ARG
1	B	348	SER
1	B	361	ASN
1	B	368	GLU
1	B	390	MET

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Mol	Chain	Res	Type
1	B	398	GLN
1	B	399	ASP
1	B	417	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	3300	GLN
1	A	3425	GLN
1	A	117	ASN
1	A	280	GLN
1	A	301	ASN
1	A	356	GLN
1	A	361	ASN
1	A	379	ASN
1	A	396	GLN
1	B	15	HIS
1	B	3301	HIS
1	B	3376	ASN
1	B	3381	ASN
1	B	117	ASN
1	B	211	GLN
1	B	231	ASN
1	B	301	ASN
1	B	356	GLN
1	B	361	ASN
1	B	378	ASN
1	B	379	ASN
1	B	396	GLN

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	$\#\|Z\| > 2$
2	AMP	A	1507	-	22,25,25	1.47	3 (13%)	25,38,38	1.92	7 (28%)
2	AMP	B	1508	-	22,25,25	1.34	3 (13%)	25,38,38	1.60	6 (24%)

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	A	1507	-	-	0/6/26/26	0/3/3/3
2	AMP	B	1508	-	-	5/6/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1507	AMP	O4'-C1'	4.29	1.47	1.41
2	B	1508	AMP	O4'-C1'	3.10	1.45	1.41
2	B	1508	AMP	C5-C4	2.98	1.48	1.40
2	B	1508	AMP	C2-N3	2.80	1.36	1.32
2	A	1507	AMP	C5-C4	2.70	1.48	1.40
2	A	1507	AMP	C2'-C1'	-2.24	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1507	AMP	C2-N1-C6	4.24	126.01	118.75
2	A	1507	AMP	O2'-C2'-C1'	-4.15	95.53	110.85
2	A	1507	AMP	N3-C2-N1	-3.50	123.21	128.68
2	B	1508	AMP	N3-C2-N1	-3.24	123.61	128.68
2	A	1507	AMP	C5-C6-N1	-3.01	113.52	120.35
2	A	1507	AMP	O3P-P-O5'	-2.86	99.12	106.73
2	B	1508	AMP	O2'-C2'-C1'	-2.60	101.24	110.85
2	A	1507	AMP	N6-C6-N1	2.42	123.60	118.57
2	B	1508	AMP	C4-C5-N7	-2.37	106.92	109.40
2	B	1508	AMP	C2-N1-C6	2.33	122.74	118.75
2	B	1508	AMP	O3P-P-O5'	-2.27	100.70	106.73
2	B	1508	AMP	P-O5'-C5'	2.15	124.23	118.30
2	A	1507	AMP	O3P-P-O1P	2.14	119.04	110.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

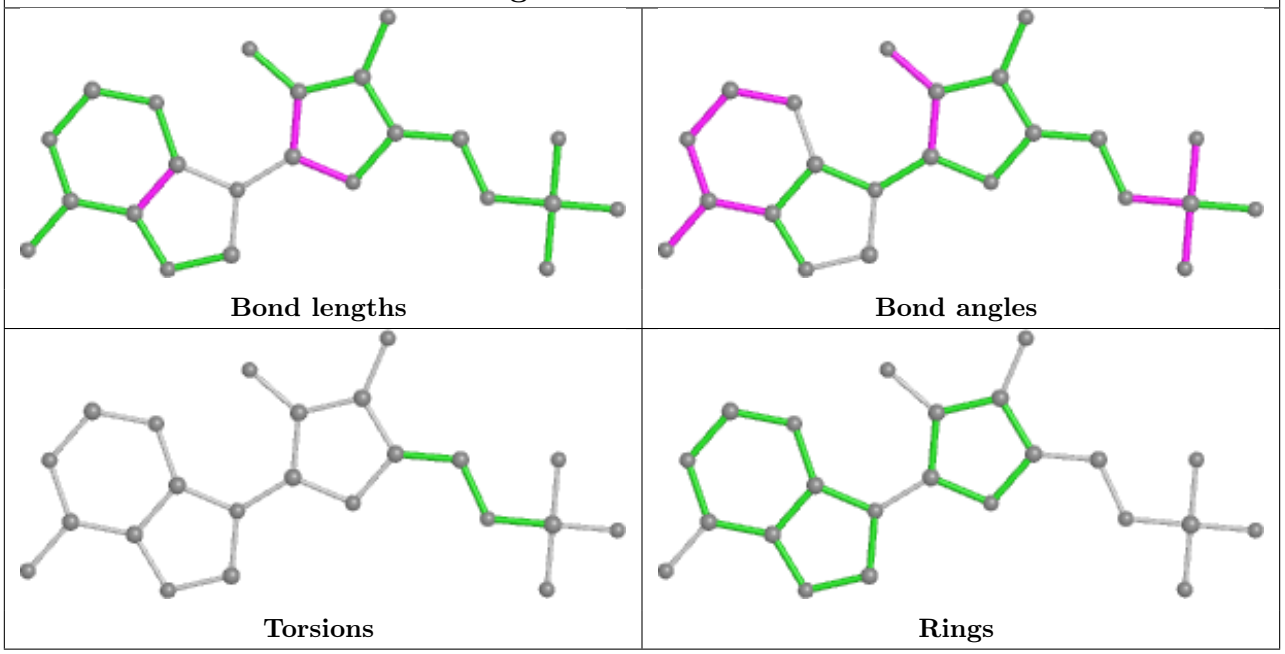
Mol	Chain	Res	Type	Atoms
2	B	1508	AMP	C5'-O5'-P-O3P
2	B	1508	AMP	O4'-C4'-C5'-O5'
2	B	1508	AMP	C3'-C4'-C5'-O5'
2	B	1508	AMP	C5'-O5'-P-O1P
2	B	1508	AMP	C5'-O5'-P-O2P

There are no ring outliers.

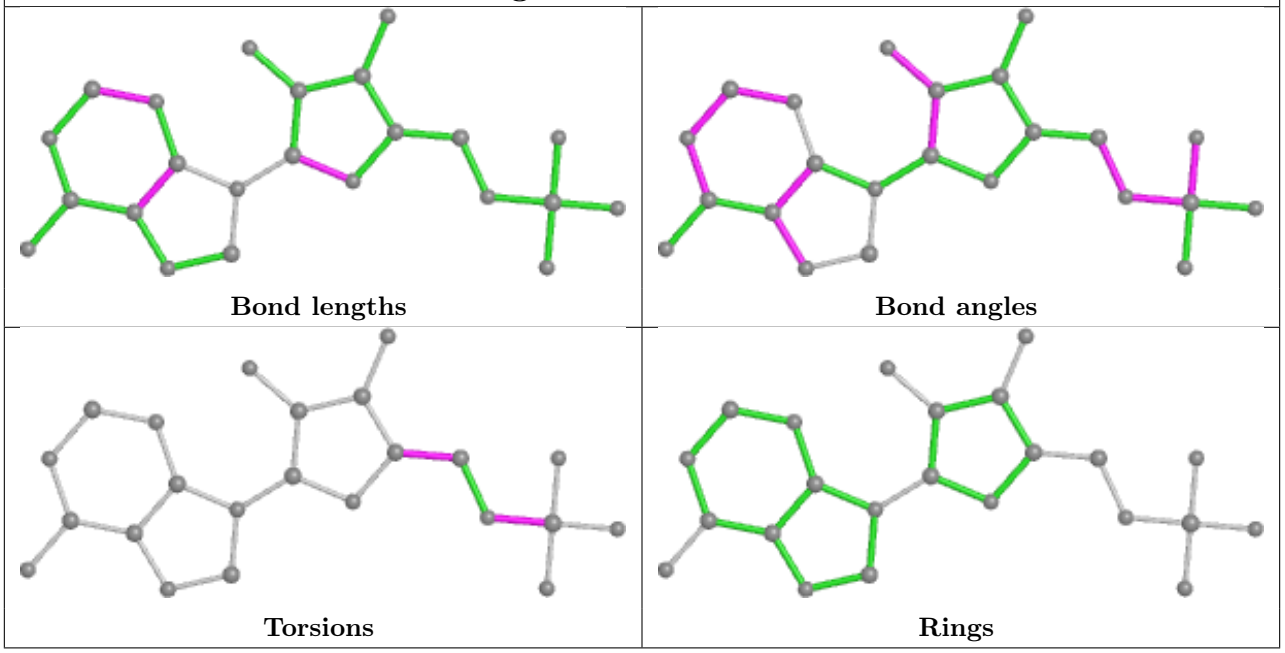
No monomer is involved in short contacts.

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 A 1507



Ligand AMP B 1508



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	527/536 (98%)	0.18	20 (3%) 40 45	23, 55, 90, 112	0
1	B	527/536 (98%)	0.48	52 (9%) 7 9	7, 68, 118, 162	0
All	All	1054/1072 (98%)	0.33	72 (6%) 17 21	7, 59, 110, 162	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3309	ALA	6.5
1	B	266	VAL	6.2
1	B	3306	ARG	6.0
1	B	3283	VAL	5.8
1	B	3276	VAL	5.5
1	A	3309	ALA	5.5
1	B	3305	VAL	5.4
1	B	12	GLU	5.3
1	B	3277	LYS	4.8
1	B	3375	TYR	4.6
1	A	370	ARG	4.5
1	A	3339	ILE	4.2
1	B	3308	MET	4.2
1	A	3303	VAL	4.1
1	A	3341	MET	4.1
1	A	3305	VAL	4.0
1	B	7	LEU	3.8
1	A	19	ARG	3.8
1	B	3274	MET	3.7
1	A	3368	ASN	3.5
1	B	262	PHE	3.5
1	B	30	LEU	3.5
1	B	3273	GLN	3.4
1	B	3268	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	3287	VAL	3.4
1	B	3380	VAL	3.2
1	B	3280	LEU	3.2
1	B	3410	LEU	3.1
1	B	3315	VAL	3.1
1	B	14	PHE	3.1
1	B	3355	GLU	3.1
1	B	3311	PRO	3.1
1	A	3330	THR	3.0
1	B	3412	ASN	3.0
1	B	3310	ASN	3.0
1	A	3355	GLU	2.7
1	A	3	ASP	2.7
1	B	11	PRO	2.7
1	B	3290	ALA	2.6
1	B	3272	LYS	2.6
1	A	419	PRO	2.6
1	B	3337	ARG	2.6
1	A	371	VAL	2.6
1	B	23	VAL	2.5
1	B	97	LEU	2.5
1	A	3342	ARG	2.5
1	A	3329	SER	2.5
1	B	3423	ASP	2.5
1	B	3269	ILE	2.4
1	B	3407	VAL	2.4
1	B	3278	GLU	2.4
1	B	3417	LEU	2.3
1	B	3422	LYS	2.3
1	B	3333	TRP	2.3
1	B	3413	GLU	2.3
1	B	3367	LYS	2.3
1	B	3307	SER	2.3
1	B	24	ALA	2.3
1	A	10	GLU	2.3
1	B	3284	GLU	2.2
1	B	3267	GLU	2.2
1	A	3302	LEU	2.2
1	B	3275	SER	2.2
1	B	3409	PRO	2.2
1	B	3314	ALA	2.1
1	A	3311	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3279	ASP	2.1
1	B	3295	LYS	2.1
1	A	3407	VAL	2.1
1	A	3297	ILE	2.1
1	B	3300	GLN	2.0
1	B	308	LEU	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)

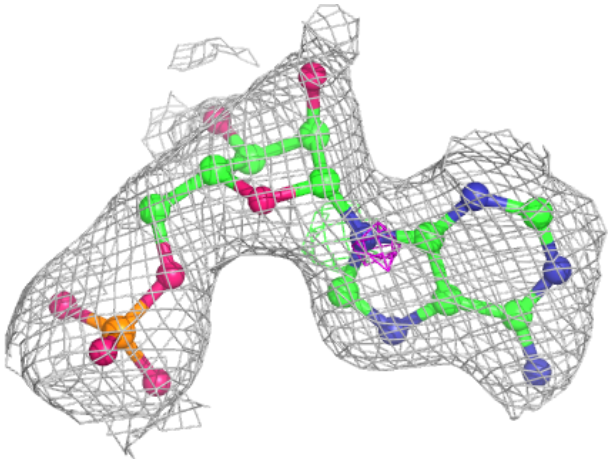
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

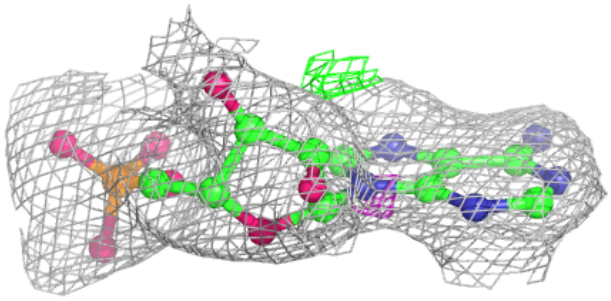
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AMP	B	1508	23/23	0.89	0.12	63,72,90,92	0
2	AMP	A	1507	23/23	0.96	0.15	36,43,66,71	0

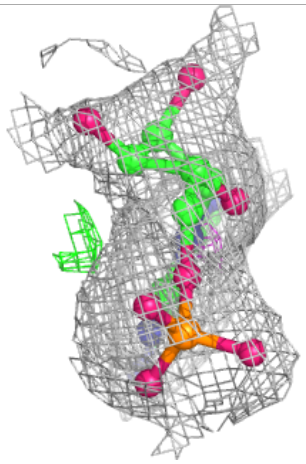
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP B 1508:

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

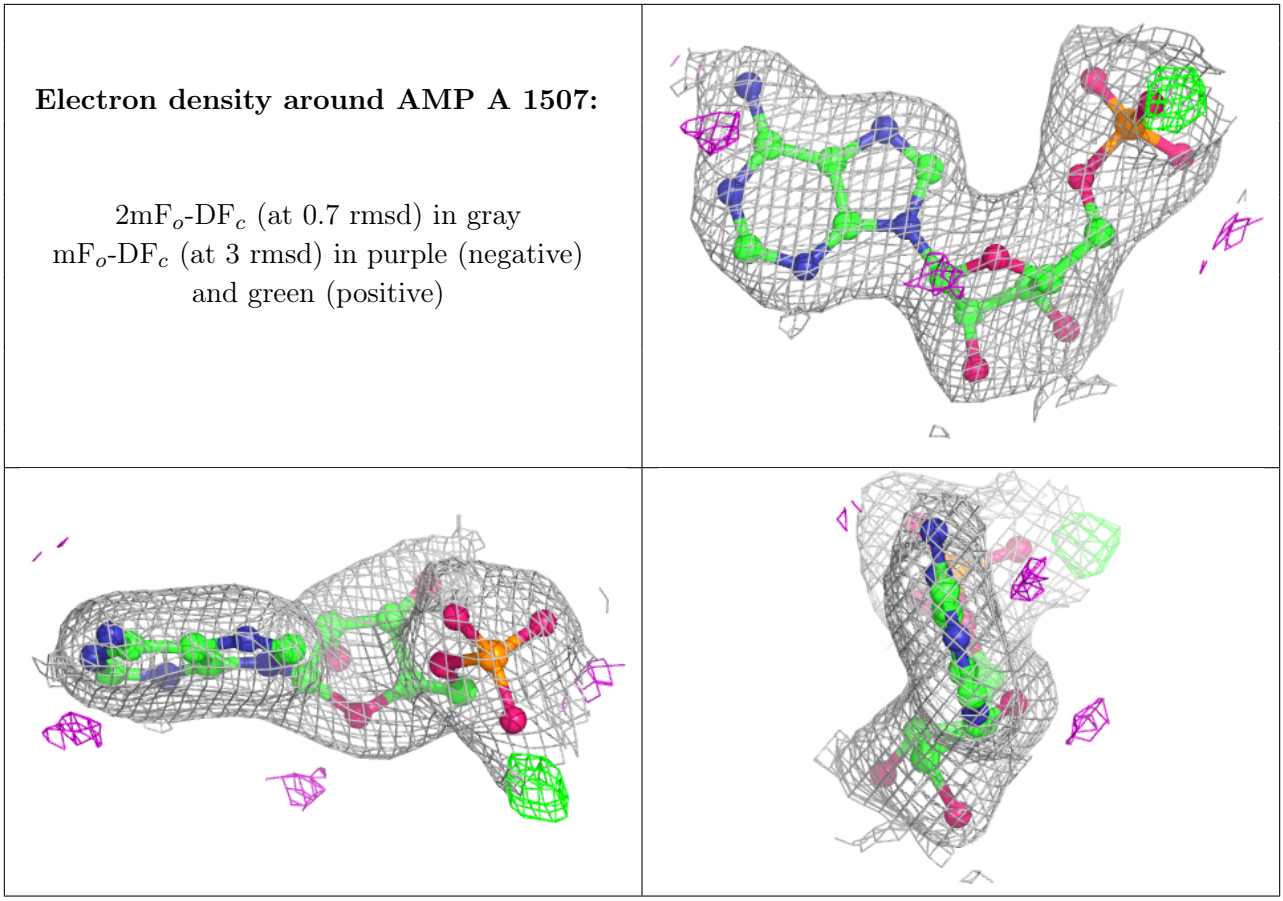






Electron density around AMP A 1507:

$2mF_o$-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.