Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 04:42 PM EDT

PDB ID	:	3PCO
Title	:	crystal structure of E. coli phenylalanine-tRNA synthetase complexed with phenylalanine and AMP
Authors	:	Mermershtain, I.; Finarov, I.; Klipcan, L.; Kessler, N.; Rozenberg, H.; Safro, M.G.
Deposited on	:	2010-10-21
Resolution	:	3.02 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:

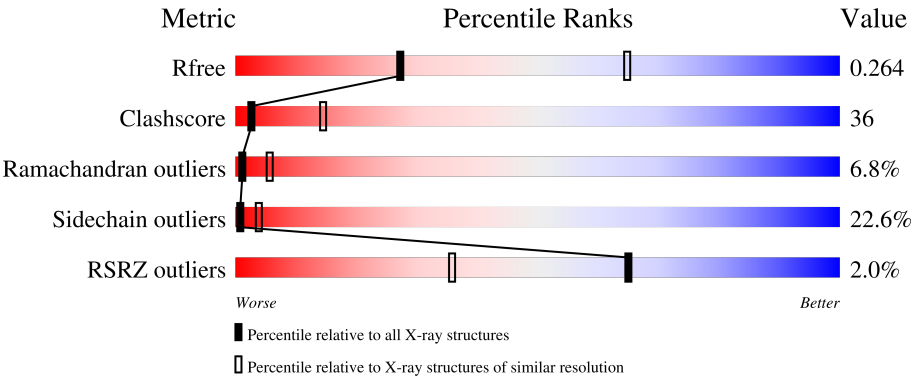
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.02 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	327	% 29% 32% 11% 26%
1	C	327	9% 43% 40% 13%
2	B	795	45% 40% 13%
2	D	795	% 46% 38% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AMP	A	992	-	-	X	-
4	AMP	C	999	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16724 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.

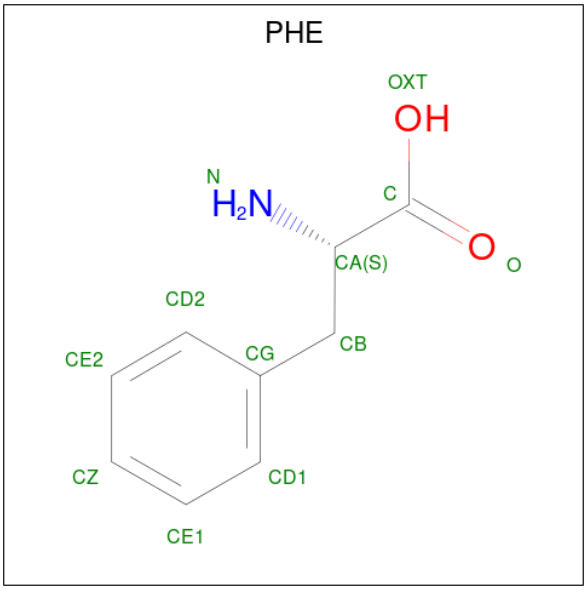
- Molecule 1 is a protein called Phenylalanyl-tRNA synthetase, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1964	1250	347	358	9			
1	C	323	Total	C	N	O	S	0	0	0
			2462	1552	445	456	9			

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase, beta chain.

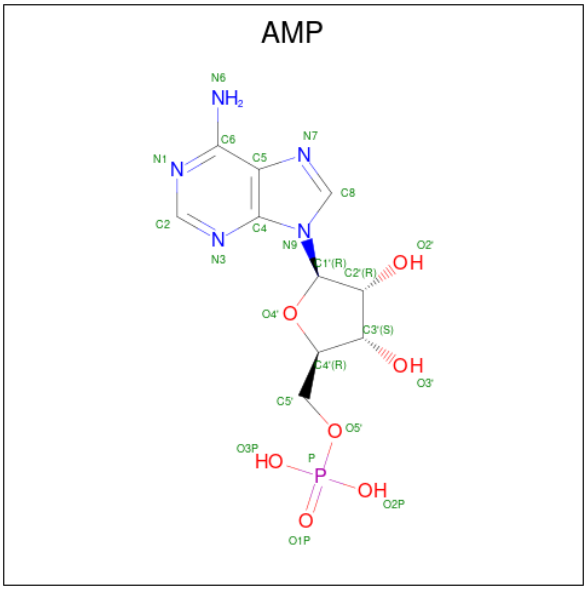
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	795	Total	C	N	O	S	0	0	0
			6111	3845	1081	1158	27			
2	D	795	Total	C	N	O	S	0	0	0
			6117	3848	1081	1161	27			

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		

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

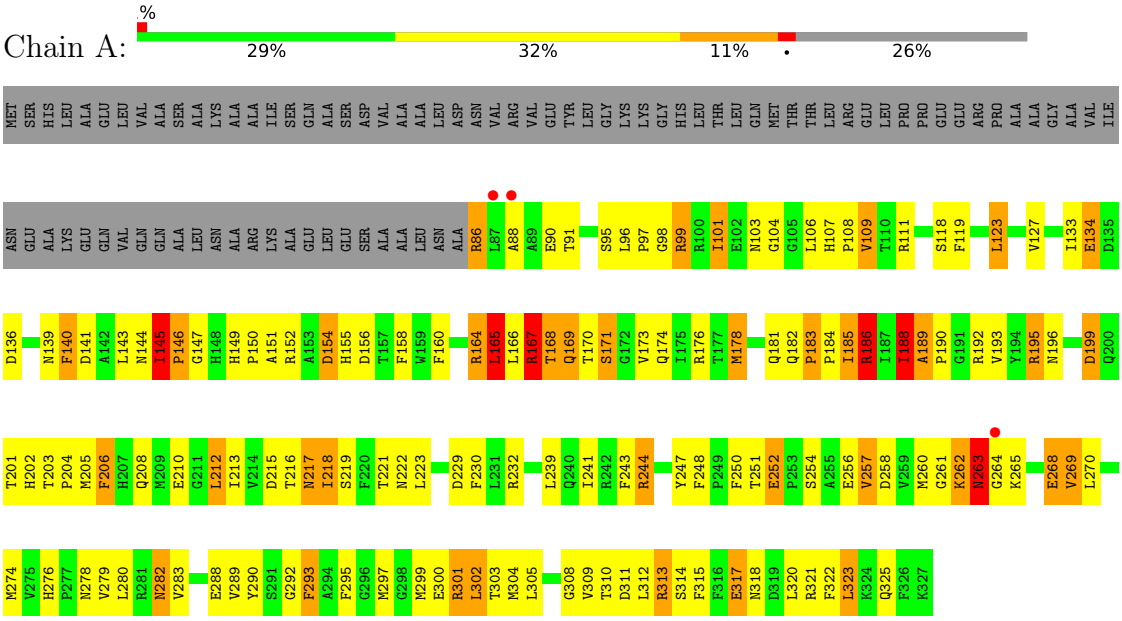


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

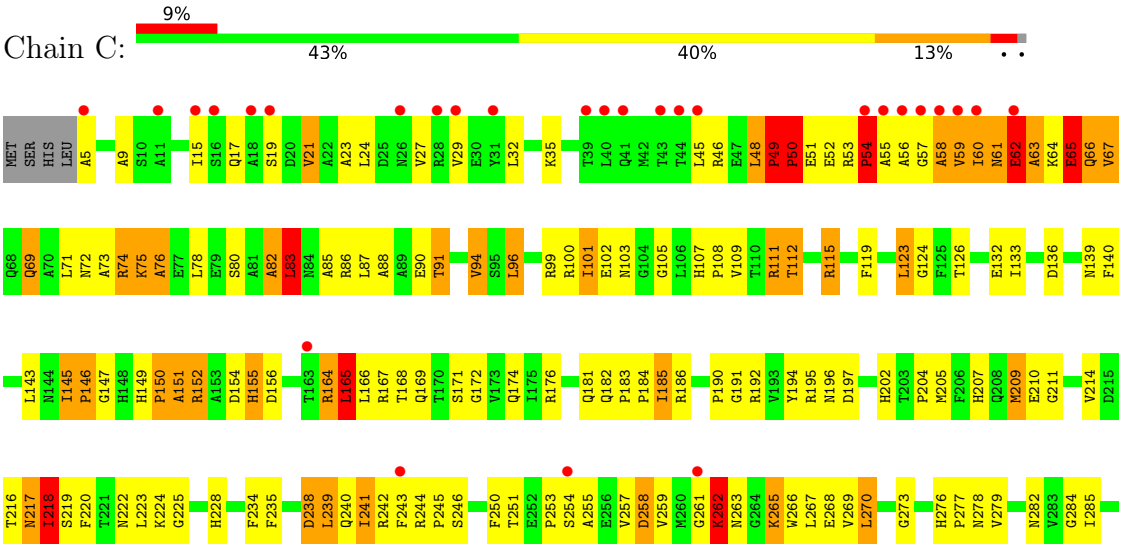
3 Residue-property plots (i)

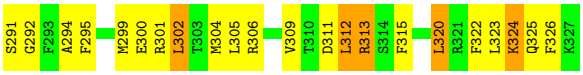
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phenylalanyl-tRNA synthetase, alpha subunit



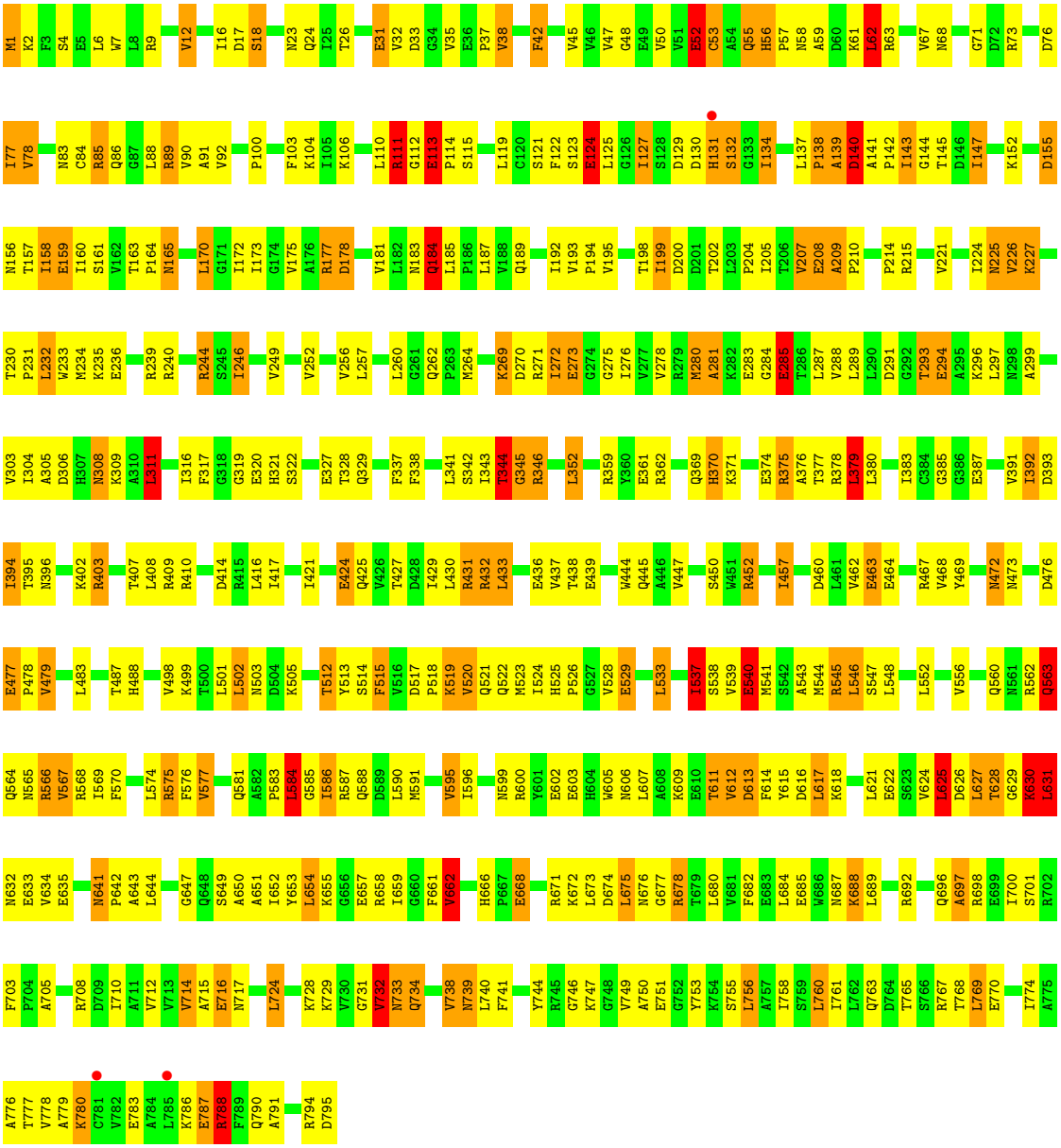
• Molecule 1: Phenylalanyl-tRNA synthetase, alpha subunit





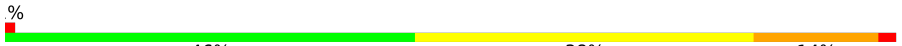
• Molecule 2: Phenylalanyl-tRNA synthetase, beta chain

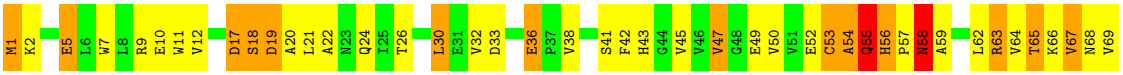
Chain B:

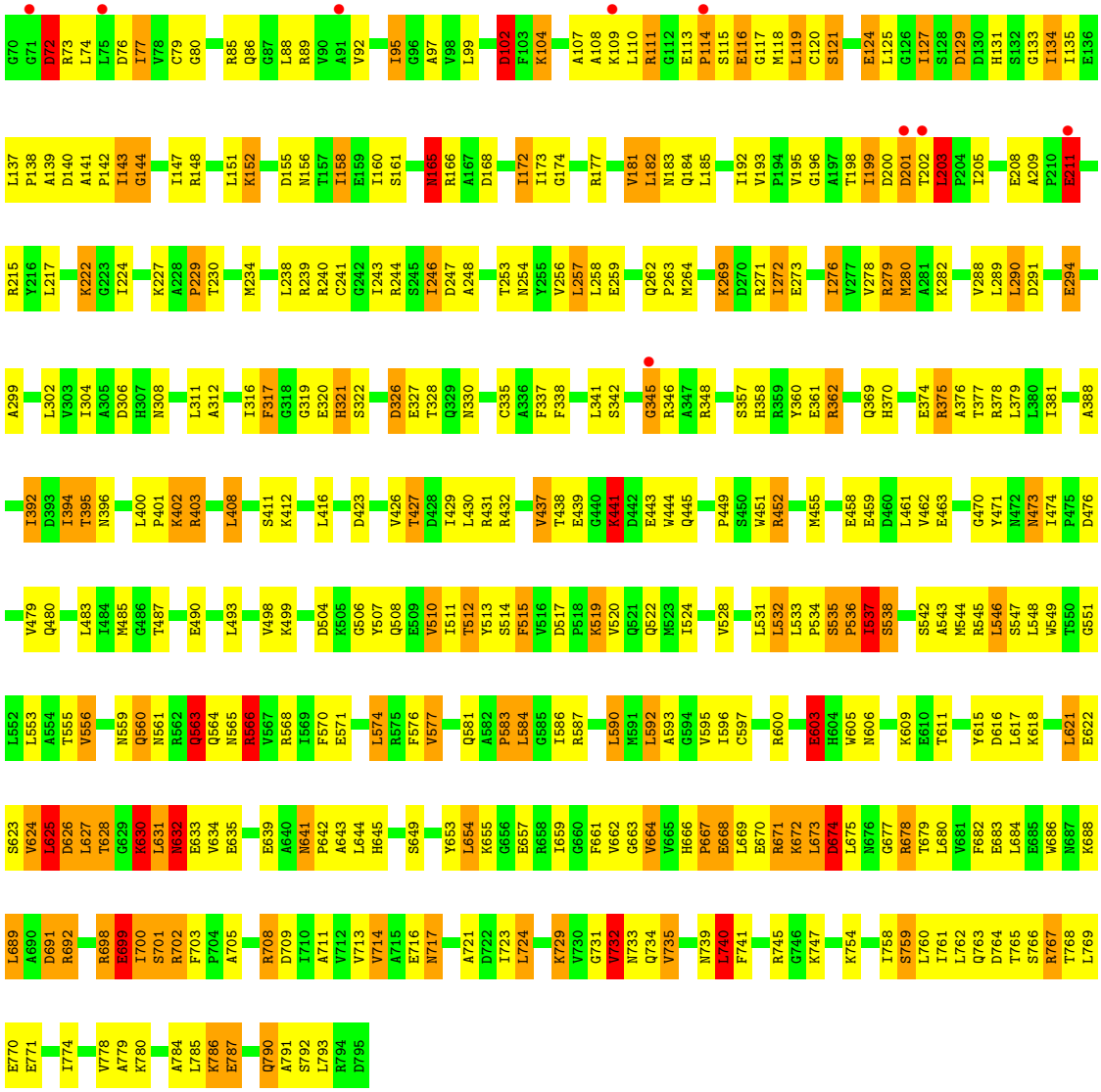


• Molecule 2: Phenylalanyl-tRNA synthetase, beta chain

Chain D:






G70 G71 D72 R73 L74 L75 D76 I77 V78 C79 G80 R85 Q86 G87 L88 R89 V90 A91 V92 I95 G96 A97 V98 L99 D102 F103 K104 A107 A108 K109 L110 R111 G112 E113 P114 S115 E116 G117 M118 L119 C120 S121 E124 L125 G126 I127 S128 D129 D130 H131 S132 G133 I134 E136
L137 P138 A139 D140 A141 P142 I143 G144 I147 R148 L151 K152 D155 N156 T157 I158 E159 I160 S161 N165 R166 A167 D168 I172 I173 G174 R177 V181 L182 N183 Q184 L185 I192 V193 P194 V195 G196 A197 T198 I199 D200 D201 T202 L203 P204 I205 E208 A209 P210 E211
R215 Y216 L217 K222 G223 I224 K227 A228 P229 T230 M234 L238 R239 R240 C241 G242 I243 R244 S245 I246 D247 A248 T253 N254 Y255 V256 V256 L257 I258 E259 Q262 P263 M264 K289 D270 R271 I272 E273 I276 V277 V278 R279 M280 A281 K282 V288 L289 L290 D291 E294
A299 L302 V303 I304 A305 D306 H307 N308 L311 A312 I316 F317 G318 G319 E320 H321 S322 D326 E327 T328 Q329 N330 C335 A336 F337 F338 L341 S342 G345 R346 A347 R348 S357 H358 R359 Y360 E361 R362 Q369 H370 E374 R375 A376 T377 R378 L379 L380 I381 A388
I392 D393 I394 T395 N396 L400 P401 K402 R403 L408 S411 K412 L416 D423 V426 T427 D428 I429 L430 R431 R432 V437 T438 E439 G440 K441 D442 E443 W444 Q445 P449 S450 W451 R452 M455 E458 E459 D460 L461 V462 E463 G470 Y471 N472 N473 I474 P475 D476
V479 Q480 L483 T484 M485 G486 T487 E490 L493 V498 K499 D504 K505 G506 Y507 Q508 E509 V510 I511 T512 Y513 S514 F515 V516 D517 P518 K519 V520 Q521 Q522 M523 I524 V528 L531 L532 L533 P534 S535 P536 I537 S538 S542 A543 M544 R545 L546 S547 L548 W549 T550 G551
L552 L553 A554 T555 V556 N559 Q560 N561 R562 Q563 Q564 N565 R566 V567 R568 I569 F570 E571 L574 R575 F576 V577 Q581 A582 P583 L584 G585 I586 R587 L590 M591 L592 A593 G594 V595 I596 C597 R600 E603 H604 W605 N606 K609 E610 T611 Y615 D616 L617 K618 L621 E622
S623 V624 K625 D626 L627 T628 G629 K630 L631 N632 E633 V634 E635 E639 A640 N641 P642 A643 L644 H645 S649 Y653 L654 K655 G656 E657 R658 I659 G660 F661 V662 G663 V664 V665 H666 P667 E668 L669 E670 R671 K672 L673 D674 L675 N676 G677 R678 T679 L680 V681 F682 E683 L684 E685 W686 N687 K688
L689 A690 D691 R692 R698 E699 I700 S701 R702 F703 P704 A705 R708 D709 I710 A711 V712 V713 V714 A715 E716 N717 A721 D722 I723 L724 K729 V730 G731 V732 N733 Q734 V735 N739 L740 F741 R745 G746 K747 K754 I758 S759 L760 T761 L762 Q763 D764 T765 S766 R767 T768 L769
E770 E771 I774 V778 A779 K780 A784 L785 K786 E787 Q790 A791 S792 L793 R794 D795

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.55Å 178.94Å 254.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.71 – 3.02 38.71 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.71-3.02) 98.4 (38.71-3.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.300 0.267 , 0.264	Depositor DCC
R_{free} test set	2981 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	75.4	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16724	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% 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

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	0.76	0/2016	0.98	5/2730 (0.2%)
1	C	0.65	0/2516	0.88	8/3412 (0.2%)
2	B	0.69	2/6212 (0.0%)	0.90	10/8432 (0.1%)
2	D	0.63	0/6218	0.84	4/8440 (0.0%)
All	All	0.67	2/16962 (0.0%)	0.89	27/23014 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
2	B	0	9
2	D	0	6
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	463	GLU	CB-CG	5.87	1.63	1.52
2	B	540	GLU	CG-CD	5.10	1.59	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	563	GLN	N-CA-C	-5.99	94.82	111.00
1	C	54	PRO	N-CA-CB	5.99	110.48	103.30
1	C	49	PRO	N-CA-CB	5.96	110.46	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	270	LEU	CA-CB-CG	5.90	128.87	115.30
1	C	50	PRO	N-CA-CB	5.82	110.29	103.30
1	A	140	PHE	CB-CA-C	-5.75	98.89	110.40
1	A	215	ASP	CB-CA-C	-5.62	99.16	110.40
2	B	533	LEU	CA-CB-CG	5.61	128.20	115.30
1	C	165	LEU	CA-CB-CG	5.60	128.17	115.30
2	B	595	VAL	CB-CA-C	-5.43	101.08	111.40
2	B	311	LEU	CA-CB-CG	5.39	127.71	115.30
2	B	379	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	165	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	96	LEU	CA-CB-CG	5.31	127.52	115.30
2	B	627	LEU	CA-CB-CG	-5.29	103.13	115.30
2	B	662	VAL	CB-CA-C	-5.28	101.36	111.40
2	D	724	LEU	CA-CB-CG	5.24	127.36	115.30
2	D	740	LEU	CA-CB-CG	5.24	127.36	115.30
2	D	119	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	312	LEU	CA-CB-CG	5.20	127.25	115.30
2	B	654	LEU	CA-CB-CG	5.19	127.23	115.30
1	C	302	LEU	N-CA-CB	5.17	120.74	110.40
1	A	301	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	167	ARG	NE-CZ-NH1	-5.07	117.76	120.30
2	B	625	LEU	CA-CB-CG	-5.04	103.71	115.30
2	B	537	ILE	CB-CA-C	-5.01	101.59	111.60
2	D	641	ASN	C-N-CD	-5.00	109.60	120.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	PRO	Peptide
2	B	113	GLU	Peptide
2	B	42	PHE	Peptide
2	B	472	ASN	Peptide
2	B	529	GLU	Peptide
2	B	55	GLN	Peptide
2	B	61	LYS	Peptide
2	B	62	LEU	Peptide
2	B	625	LEU	Peptide
2	B	631	LEU	Peptide
1	C	182	GLN	Peptide
1	C	183	PRO	Peptide
1	C	262	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	D	246	ILE	Peptide
2	D	345	GLY	Peptide
2	D	55	GLN	Peptide
2	D	58	ASN	Peptide
2	D	672	LYS	Peptide
2	D	72	ASP	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	1964	0	1900	213	0
1	C	2462	0	2307	217	0
2	B	6111	0	6166	419	0
2	D	6117	0	6169	430	0
3	A	12	0	8	2	0
3	C	12	0	8	1	0
4	A	23	0	12	9	0
4	C	23	0	12	9	0
All	All	16724	0	16582	1211	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 36.

All (1211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:GLN:HB2	2:D:56:HIS:CA	1.37	1.46
1:C:58:ALA:C	1:C:60:ILE:HB	1.48	1.34
1:C:58:ALA:HB1	1:C:60:ILE:CG2	1.58	1.33
2:D:631:LEU:HD12	2:D:632:ASN:N	1.47	1.27
2:D:55:GLN:HB2	2:D:56:HIS:C	1.56	1.24
1:A:155:HIS:CD2	1:A:168:THR:HG21	1.76	1.19
1:A:185:ILE:CD1	1:A:212:LEU:HD13	1.72	1.19
1:C:58:ALA:O	1:C:59:VAL:HG12	1.43	1.18
1:C:239:LEU:HB3	1:C:240:GLN:HA	1.24	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:CE2	1:A:195:ARG:O	1.97	1.17
2:D:56:HIS:HB3	2:D:57:PRO:HA	1.17	1.16
1:A:170:THR:O	1:A:210:GLU:HG3	1.42	1.16
1:C:62:GLU:HG3	1:C:63:ALA:H	1.05	1.15
1:A:140:PHE:O	1:A:145:ILE:HG12	1.47	1.14
2:D:56:HIS:CE1	2:D:58:ASN:HB3	1.82	1.14
2:D:115:SER:O	2:D:116:GLU:O	1.65	1.13
1:C:60:ILE:HG22	1:C:61:ASN:H	0.97	1.13
2:D:375:ARG:HG3	2:D:375:ARG:HH11	1.02	1.12
1:A:104:GLY:O	2:B:503:ASN:CG	1.88	1.12
2:D:631:LEU:CD1	2:D:632:ASN:H	1.62	1.12
2:B:522:GLN:NE2	2:B:529:GLU:HG3	1.65	1.12
2:B:537:ILE:H	2:B:537:ILE:HD12	0.98	1.12
1:A:145:ILE:HB	1:A:146:PRO:HA	1.31	1.11
1:C:59:VAL:N	1:C:60:ILE:HB	1.63	1.11
1:A:185:ILE:HD11	1:A:212:LEU:HD13	1.26	1.09
1:A:88:ALA:O	1:A:91:THR:HG23	1.49	1.09
1:C:58:ALA:CB	1:C:60:ILE:CG2	2.30	1.09
2:D:55:GLN:HB2	2:D:56:HIS:HA	1.20	1.09
2:D:55:GLN:CB	2:D:56:HIS:CA	2.30	1.08
2:B:452:ARG:HH11	2:B:452:ARG:HG2	1.00	1.07
1:C:60:ILE:CG2	1:C:61:ASN:H	1.66	1.07
1:C:62:GLU:HG3	1:C:63:ALA:N	1.62	1.07
1:A:166:LEU:O	1:A:167:ARG:O	1.70	1.07
1:C:60:ILE:HG22	1:C:61:ASN:N	1.64	1.06
1:A:166:LEU:HD11	2:B:544:MET:CE	1.83	1.05
2:B:522:GLN:HE22	2:B:529:GLU:CG	1.67	1.05
2:D:452:ARG:HG2	2:D:452:ARG:HH11	1.18	1.04
2:B:631:LEU:HG	2:B:632:ASN:H	1.17	1.04
2:D:55:GLN:CB	2:D:56:HIS:O	2.06	1.04
1:C:59:VAL:HA	1:C:60:ILE:O	1.59	1.03
2:B:787:GLU:O	2:B:788:ARG:HD2	1.58	1.03
2:D:56:HIS:CB	2:D:57:PRO:HA	1.88	1.03
2:D:449:PRO:HD2	2:D:455:MET:HE1	1.40	1.02
1:C:58:ALA:CA	1:C:60:ILE:HB	1.90	1.01
2:B:522:GLN:HE22	2:B:529:GLU:HG3	0.88	1.01
2:B:537:ILE:H	2:B:537:ILE:CD1	1.73	1.00
1:A:136:ASP:OD1	1:A:152:ARG:NH2	1.95	1.00
2:B:600:ARG:NH1	2:B:616:ASP:OD2	1.94	1.00
1:A:164:ARG:NH1	2:B:585:GLY:H	1.58	0.99
1:C:58:ALA:HB1	1:C:60:ILE:HG22	0.98	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HA	1:A:282:ASN:HD21	1.26	0.98
1:A:164:ARG:HH12	2:B:585:GLY:H	1.05	0.98
2:D:625:LEU:O	2:D:626:ASP:CB	2.12	0.97
1:A:139:ASN:HD21	1:A:168:THR:HB	1.27	0.97
2:D:55:GLN:CB	2:D:56:HIS:C	2.31	0.97
2:D:732:VAL:HG13	2:D:733:ASN:H	1.26	0.97
2:D:269:LYS:O	2:D:272:ILE:HD12	1.65	0.97
1:A:140:PHE:C	1:A:145:ILE:HG12	1.84	0.96
2:D:375:ARG:HH11	2:D:375:ARG:CG	1.78	0.96
1:A:166:LEU:HD11	2:B:544:MET:HE3	1.48	0.96
2:B:244:ARG:H	2:B:244:ARG:HE	1.10	0.96
1:C:58:ALA:CB	1:C:60:ILE:HG22	1.92	0.95
1:A:222:ASN:HB3	2:B:479:VAL:HG12	1.47	0.95
2:B:630:LYS:HB3	2:B:631:LEU:O	1.66	0.95
2:D:631:LEU:HD12	2:D:632:ASN:H	0.79	0.94
2:D:716:GLU:OE1	2:D:745:ARG:NH1	2.00	0.94
1:A:188:ILE:O	1:A:189:ALA:HB2	1.65	0.94
1:A:168:THR:HG22	1:A:169:GLN:HG3	1.47	0.94
2:B:644:LEU:HD13	2:B:649:SER:HB2	1.50	0.94
2:D:253:THR:HG22	2:D:264:MET:HB2	1.48	0.94
1:C:59:VAL:N	1:C:60:ILE:CB	2.30	0.93
2:B:631:LEU:CG	2:B:632:ASN:H	1.81	0.93
2:B:600:ARG:NH1	2:B:616:ASP:OD1	2.02	0.93
1:C:276:HIS:HD2	1:C:278:ASN:HB2	1.33	0.93
2:D:26:THR:HG22	2:D:32:VAL:H	1.34	0.93
1:C:202:HIS:CE1	1:C:301:ARG:HH22	1.85	0.93
2:B:452:ARG:HG2	2:B:452:ARG:NH1	1.76	0.92
1:C:75:LYS:HG3	1:C:75:LYS:O	1.67	0.92
2:D:632:ASN:OD1	2:D:633:GLU:HG2	1.68	0.92
2:D:55:GLN:CB	2:D:56:HIS:HA	1.98	0.91
2:D:499:LYS:HD3	2:D:570:PHE:HE1	1.33	0.91
2:B:537:ILE:HD12	2:B:537:ILE:N	1.84	0.91
2:D:577:VAL:HG13	2:D:587:ARG:HB3	1.52	0.91
2:D:626:ASP:O	2:D:628:THR:N	2.05	0.90
2:B:586:ILE:H	2:B:586:ILE:HD12	1.35	0.90
2:D:53:CYS:O	2:D:53:CYS:SG	2.30	0.90
2:B:78:VAL:HG12	2:B:115:SER:HB3	1.52	0.90
1:A:203:THR:H	4:A:992:AMP:HN61	1.20	0.89
2:D:786:LYS:HD2	2:D:791:ALA:HB3	1.53	0.89
2:B:596:ILE:HD12	2:B:612:VAL:HG21	1.53	0.88
1:A:145:ILE:CB	1:A:146:PRO:HA	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:HIS:HD2	1:A:168:THR:HG21	1.29	0.88
2:B:111:ARG:N	2:B:112:GLY:HA2	1.89	0.88
2:B:600:ARG:NH1	2:B:616:ASP:CG	2.27	0.88
2:B:668:GLU:N	2:B:668:GLU:OE1	2.06	0.88
2:D:517:ASP:HB3	2:D:520:VAL:HB	1.55	0.87
2:B:344:THR:HA	2:B:361:GLU:OE1	1.75	0.87
2:B:625:LEU:O	2:B:627:LEU:N	2.08	0.87
2:B:205:ILE:HG22	2:B:276:ILE:HB	1.54	0.87
2:D:375:ARG:HG3	2:D:375:ARG:NH1	1.84	0.87
2:D:634:VAL:HG22	2:D:654:LEU:HB2	1.55	0.87
1:A:166:LEU:O	1:A:167:ARG:C	2.12	0.86
1:C:54:PRO:N	1:C:55:ALA:HA	1.89	0.86
1:A:104:GLY:O	2:B:503:ASN:CB	2.23	0.86
1:C:58:ALA:CB	1:C:60:ILE:HG21	2.04	0.85
2:B:710:ILE:HD13	2:B:712:VAL:HG23	1.55	0.85
1:C:195:ARG:O	1:C:204:PRO:HA	1.77	0.85
1:A:95:SER:HB2	2:D:721:ALA:HB2	1.59	0.85
1:A:145:ILE:HB	1:A:146:PRO:CA	2.06	0.84
2:B:165:ASN:HD22	2:B:165:ASN:H	1.24	0.84
2:D:701:SER:HA	2:D:702:ARG:HH21	1.42	0.84
2:D:177:ARG:O	2:D:181:VAL:HG12	1.77	0.84
2:D:700:ILE:O	2:D:701:SER:HB3	1.77	0.84
1:C:107:HIS:HE1	1:C:109:VAL:HG13	1.43	0.84
2:D:113:GLU:HB3	2:D:114:PRO:HD2	1.58	0.83
1:A:140:PHE:CA	1:A:145:ILE:HG12	2.07	0.83
1:C:202:HIS:CE1	1:C:301:ARG:NH2	2.45	0.83
2:D:627:LEU:HD11	2:D:631:LEU:HD23	1.61	0.83
1:C:62:GLU:CG	1:C:63:ALA:N	2.42	0.83
2:D:205:ILE:HG22	2:D:276:ILE:HB	1.60	0.82
1:A:300:GLU:HB3	1:A:312:LEU:CD1	2.10	0.82
1:C:59:VAL:N	1:C:60:ILE:C	2.33	0.82
2:D:626:ASP:C	2:D:628:THR:H	1.80	0.82
1:C:224:LYS:HE2	2:D:474:ILE:O	1.78	0.82
2:B:343:ILE:O	2:B:346:ARG:HG2	1.80	0.81
2:D:85:ARG:HB3	2:D:88:LEU:HD13	1.62	0.81
2:B:432:ARG:HG2	2:B:432:ARG:HH11	1.44	0.81
2:D:515:PHE:HD1	2:D:544:MET:HE1	1.46	0.81
1:A:166:LEU:HD11	2:B:544:MET:HE1	1.60	0.81
1:A:140:PHE:O	1:A:145:ILE:CG1	2.27	0.81
1:C:59:VAL:H	1:C:60:ILE:C	1.84	0.81
1:C:59:VAL:HG13	1:C:59:VAL:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:HG22	2:B:432:ARG:HG3	1.63	0.80
2:B:631:LEU:HG	2:B:632:ASN:N	1.96	0.80
2:D:45:VAL:HB	2:D:147:ILE:HD11	1.62	0.80
2:D:55:GLN:HB3	2:D:56:HIS:O	1.80	0.80
2:B:429:ILE:HG23	2:B:468:VAL:HG21	1.63	0.80
1:C:59:VAL:HG23	1:C:62:GLU:HG2	1.61	0.80
1:C:59:VAL:CA	1:C:60:ILE:C	2.50	0.80
2:D:510:VAL:O	2:D:571:GLU:HG3	1.80	0.80
2:D:626:ASP:C	2:D:628:THR:N	2.32	0.80
2:B:651:ALA:HB1	2:B:658:ARG:HD3	1.64	0.79
2:D:644:LEU:HD13	2:D:649:SER:HB2	1.64	0.79
1:A:185:ILE:HD12	1:A:212:LEU:HD13	1.64	0.79
2:D:790:GLN:HE21	2:D:791:ALA:H	1.29	0.79
1:C:58:ALA:CA	1:C:60:ILE:CB	2.61	0.79
2:D:56:HIS:HB3	2:D:57:PRO:CA	2.07	0.79
2:B:244:ARG:HE	2:B:244:ARG:N	1.79	0.79
2:D:733:ASN:HA	2:D:734:GLN:HB2	1.63	0.79
2:D:357:SER:O	2:D:361:GLU:HG2	1.82	0.79
2:B:285:GLU:HB2	2:B:297:LEU:HB2	1.65	0.78
1:C:59:VAL:CA	1:C:60:ILE:O	2.31	0.78
2:D:56:HIS:CE1	2:D:58:ASN:CB	2.64	0.78
1:A:203:THR:H	4:A:992:AMP:N6	1.81	0.78
1:A:149:HIS:CG	1:A:150:PRO:HD2	2.18	0.78
1:A:300:GLU:HB3	1:A:312:LEU:HD13	1.66	0.78
2:D:85:ARG:HB3	2:D:88:LEU:CD1	2.13	0.78
1:A:155:HIS:CD2	1:A:168:THR:CG2	2.63	0.77
2:B:85:ARG:NH2	2:B:88:LEU:HD11	1.99	0.77
1:C:107:HIS:CE1	1:C:109:VAL:HG13	2.20	0.77
2:D:209:ALA:HB1	2:D:211:GLU:OE2	1.84	0.77
2:B:198:THR:O	2:B:199:ILE:HG23	1.84	0.77
1:A:147:GLY:HA2	1:A:152:ARG:NE	2.00	0.77
1:A:270:LEU:HB3	1:A:297:MET:HB3	1.66	0.77
1:A:139:ASN:O	1:A:143:LEU:HD12	1.84	0.77
2:B:560:GLN:HE22	2:B:675:LEU:HA	1.49	0.77
2:D:32:VAL:HB	2:D:158:ILE:HD11	1.66	0.77
2:B:56:HIS:HB3	2:B:63:ARG:H	1.51	0.76
2:D:641:ASN:O	2:D:643:ALA:N	2.18	0.76
2:B:272:ILE:HG12	2:B:273:GLU:N	2.00	0.76
1:A:164:ARG:HH12	2:B:585:GLY:N	1.83	0.76
2:B:9:ARG:HA	2:B:12:VAL:O	1.86	0.76
2:B:272:ILE:HG12	2:B:273:GLU:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:GLY:O	2:D:321:HIS:N	2.18	0.76
1:C:239:LEU:HB3	1:C:240:GLN:CA	2.13	0.75
2:B:600:ARG:HH11	2:B:616:ASP:CG	1.89	0.75
1:A:188:ILE:O	1:A:189:ALA:CB	2.33	0.75
2:D:618:LYS:O	2:D:622:GLU:HB2	1.86	0.75
2:B:38:VAL:HG21	2:B:240:ARG:HD3	1.69	0.74
1:C:58:ALA:O	1:C:59:VAL:CG1	2.30	0.74
1:C:59:VAL:N	1:C:60:ILE:CA	2.49	0.74
1:A:276:HIS:HD2	1:A:278:ASN:H	1.35	0.74
2:D:784:ALA:O	2:D:787:GLU:HB3	1.87	0.74
1:A:304:MET:HG2	1:A:309:VAL:O	1.88	0.74
2:B:202:THR:HG21	2:B:392:ILE:HD11	1.69	0.74
2:D:473:ASN:H	2:D:473:ASN:ND2	1.86	0.74
2:B:425:GLN:O	2:B:429:ILE:HG12	1.88	0.74
1:C:62:GLU:O	1:C:64:LYS:N	2.21	0.74
2:B:393:ASP:OD2	2:B:395:THR:HG23	1.87	0.74
2:D:499:LYS:HD3	2:D:570:PHE:CE1	2.20	0.74
1:A:145:ILE:CB	1:A:146:PRO:CA	2.61	0.73
2:B:710:ILE:CD1	2:B:712:VAL:HG23	2.17	0.73
3:A:980:PHE:N	4:A:992:AMP:HO3'	1.86	0.73
2:B:341:LEU:HD12	2:B:341:LEU:H	1.53	0.73
2:D:624:VAL:HG12	2:D:625:LEU:N	2.02	0.73
1:A:263:ASN:HB3	1:A:264:GLY:CA	2.18	0.73
1:C:276:HIS:CD2	1:C:278:ASN:HB2	2.22	0.73
2:D:168:ASP:O	2:D:174:GLY:HA3	1.88	0.73
2:B:515:PHE:HD1	2:B:544:MET:HE1	1.54	0.73
2:B:631:LEU:CG	2:B:632:ASN:N	2.51	0.73
1:C:146:PRO:O	1:C:152:ARG:NE	2.21	0.73
1:A:136:ASP:CG	1:A:152:ARG:HH22	1.91	0.72
1:A:216:THR:O	1:A:217:ASN:HB2	1.88	0.72
1:C:239:LEU:CB	1:C:240:GLN:HA	2.12	0.72
1:A:95:SER:HB2	2:D:721:ALA:CB	2.18	0.72
1:C:87:LEU:O	1:C:91:THR:HG22	1.89	0.72
1:A:104:GLY:O	2:B:503:ASN:HB3	1.89	0.72
2:D:631:LEU:CD1	2:D:632:ASN:N	2.35	0.72
2:D:273:GLU:HG3	2:D:306:ASP:OD1	1.90	0.72
2:D:626:ASP:CB	2:D:631:LEU:HD22	2.19	0.72
2:D:127:ILE:C	2:D:127:ILE:HD13	2.10	0.72
2:D:702:ARG:H	2:D:702:ARG:NE	1.88	0.72
2:B:47:VAL:HG21	2:B:141:ALA:HB1	1.70	0.71
2:B:432:ARG:HH11	2:B:432:ARG:CG	2.01	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLN:HE21	1:C:69:GLN:HA	1.55	0.71
2:D:596:ILE:HG13	2:D:680:LEU:HB2	1.72	0.71
2:D:57:PRO:HB3	2:D:59:ALA:O	1.90	0.71
2:B:111:ARG:H	2:B:112:GLY:HA2	1.56	0.71
1:A:218:ILE:HD13	1:A:293:PHE:CD1	2.26	0.71
2:D:699:GLU:HA	2:D:699:GLU:OE1	1.90	0.71
2:D:338:PHE:HD2	2:D:360:TYR:CE1	2.09	0.70
1:C:299:MET:HE2	1:C:299:MET:HA	1.73	0.70
2:D:47:VAL:HG23	2:D:142:PRO:O	1.91	0.70
1:A:170:THR:OG1	1:A:210:GLU:HG2	1.91	0.70
2:B:626:ASP:CA	2:B:629:GLY:H	2.05	0.70
2:D:22:ALA:HB1	2:D:32:VAL:HG21	1.72	0.70
2:D:193:VAL:O	2:D:378:ARG:NH1	2.24	0.70
2:B:119:LEU:HB3	2:B:134:ILE:HG21	1.73	0.70
2:D:243:ILE:HG13	2:D:258:LEU:HD11	1.73	0.70
1:C:66:GLN:HG2	1:C:67:VAL:N	2.06	0.70
2:D:119:LEU:HB3	2:D:134:ILE:HD11	1.72	0.70
2:D:394:ILE:HG13	2:D:394:ILE:O	1.92	0.70
2:D:534:PRO:O	2:D:535:SER:HB3	1.92	0.70
2:D:732:VAL:HG13	2:D:733:ASN:N	2.05	0.70
1:A:145:ILE:HG22	1:A:146:PRO:C	2.13	0.69
1:C:58:ALA:CA	1:C:60:ILE:CG2	2.70	0.69
2:D:195:VAL:HG21	2:D:377:THR:HB	1.74	0.69
2:B:522:GLN:NE2	2:B:529:GLU:CG	2.41	0.69
1:C:185:ILE:HD13	1:C:186:ARG:N	2.08	0.69
1:A:263:ASN:HB3	1:A:264:GLY:HA2	1.74	0.69
1:A:158:PHE:HZ	2:B:537:ILE:HG13	1.58	0.69
1:A:145:ILE:CG2	1:A:146:PRO:O	2.40	0.69
1:A:140:PHE:CD1	1:A:145:ILE:HG13	2.29	0.68
2:B:205:ILE:CG2	2:B:276:ILE:HB	2.24	0.68
1:C:60:ILE:CG2	1:C:61:ASN:N	2.34	0.68
2:B:605:TRP:HB3	2:D:740:LEU:HD12	1.76	0.68
2:D:791:ALA:HB1	2:D:792:SER:CB	2.23	0.68
2:B:429:ILE:HG22	2:B:433:LEU:CD2	2.24	0.68
2:B:215:ARG:HE	2:B:395:THR:HG22	1.58	0.68
2:D:253:THR:HG22	2:D:264:MET:CB	2.22	0.68
2:B:272:ILE:CG1	2:B:273:GLU:H	2.05	0.68
2:B:609:LYS:O	2:B:609:LYS:HG2	1.93	0.68
1:A:279:VAL:HA	1:A:282:ASN:ND2	2.06	0.68
2:B:165:ASN:HD22	2:B:165:ASN:N	1.90	0.68
2:B:56:HIS:HB3	2:B:63:ARG:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:CZ	2:B:537:ILE:HG13	2.29	0.67
2:B:429:ILE:HG22	2:B:433:LEU:HD22	1.76	0.67
2:B:596:ILE:HD12	2:B:612:VAL:CG2	2.25	0.67
2:D:345:GLY:H	2:D:346:ARG:HH11	1.43	0.67
2:D:427:THR:HG22	2:D:444:TRP:HE1	1.59	0.67
2:D:512:THR:HG21	2:D:551:GLY:HA3	1.75	0.67
2:B:617:LEU:HD12	2:B:680:LEU:HB3	1.76	0.67
2:D:512:THR:HB	2:D:571:GLU:OE1	1.94	0.67
1:A:169:GLN:HA	1:A:193:VAL:HG11	1.76	0.67
2:B:403:ARG:HH21	2:B:450:SER:HB3	1.61	0.67
1:A:311:ASP:OD1	1:A:313:ARG:HG3	1.95	0.66
2:B:763:GLN:HA	2:B:769:LEU:HD11	1.77	0.66
1:C:61:ASN:O	1:C:62:GLU:C	2.33	0.66
2:D:57:PRO:HG3	2:D:63:ARG:HH12	1.59	0.66
2:D:673:LEU:O	2:D:674:ASP:O	2.13	0.66
2:B:24:GLN:HE22	2:B:183:ASN:CG	1.98	0.66
2:B:647:GLY:CA	1:C:91:THR:HB	2.25	0.66
2:B:42:PHE:HB3	2:B:100:PRO:HD3	1.77	0.66
2:D:701:SER:HA	2:D:702:ARG:NH2	2.11	0.66
1:C:58:ALA:HA	1:C:60:ILE:CB	2.25	0.66
2:D:116:GLU:OE1	2:D:117:GLY:HA3	1.96	0.66
1:A:166:LEU:C	1:A:167:ARG:O	2.34	0.66
2:D:703:PHE:CE2	2:D:766:SER:O	2.49	0.65
1:A:107:HIS:CD2	1:A:109:VAL:H	2.15	0.65
1:C:214:VAL:HG22	1:C:292:GLY:HA3	1.77	0.65
2:B:701:SER:HB3	2:B:765:THR:HA	1.77	0.65
1:A:134:GLU:OE2	1:A:134:GLU:HA	1.96	0.65
2:D:596:ILE:HG12	2:D:617:LEU:HD13	1.78	0.65
1:A:170:THR:O	1:A:210:GLU:CG	2.33	0.65
2:D:64:VAL:CG2	2:D:114:PRO:HG2	2.26	0.65
2:D:770:GLU:O	2:D:774:ILE:HG12	1.96	0.65
1:A:178:MET:CE	1:A:280:LEU:HD23	2.26	0.65
2:D:32:VAL:HA	2:D:160:ILE:HG22	1.78	0.65
1:A:260:MET:SD	1:A:265:LYS:HE3	2.37	0.65
2:B:139:ALA:C	2:B:141:ALA:H	2.00	0.65
1:C:61:ASN:O	1:C:63:ALA:N	2.30	0.65
1:C:59:VAL:H	1:C:61:ASN:N	1.95	0.65
1:C:299:MET:HA	1:C:299:MET:CE	2.27	0.65
2:D:259:GLU:OE1	2:D:375:ARG:NH1	2.29	0.65
1:A:229:ASP:OD1	1:A:232:ARG:NH2	2.31	0.64
2:D:624:VAL:CG1	2:D:625:LEU:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:VAL:HA	1:C:60:ILE:C	2.16	0.64
2:D:64:VAL:HG23	2:D:114:PRO:HG2	1.80	0.64
1:A:133:ILE:HD12	2:B:576:PHE:CD1	2.32	0.64
2:B:139:ALA:O	2:B:141:ALA:N	2.30	0.64
2:B:225:ASN:H	2:B:385:GLY:H	1.45	0.64
2:B:586:ILE:HD12	2:B:586:ILE:N	2.05	0.64
2:D:624:VAL:HG12	2:D:625:LEU:H	1.58	0.64
2:B:62:LEU:HB2	2:B:63:ARG:HD2	1.79	0.64
2:B:305:ALA:HA	2:B:311:LEU:HD13	1.79	0.64
1:C:192:ARG:HG3	1:C:207:HIS:CE1	2.33	0.64
2:D:717:ASN:ND2	2:D:717:ASN:O	2.30	0.64
2:B:311:LEU:O	2:B:319:GLY:HA3	1.98	0.64
2:B:452:ARG:HH11	2:B:452:ARG:CG	1.92	0.64
2:D:166:ARG:O	2:D:166:ARG:HG3	1.96	0.64
2:D:192:ILE:HG12	2:D:375:ARG:HG2	1.80	0.64
2:B:55:GLN:O	2:B:56:HIS:ND1	2.31	0.64
2:B:427:THR:HG21	2:B:439:GLU:CD	2.18	0.64
2:B:462:VAL:O	2:B:463:GLU:C	2.35	0.64
2:D:624:VAL:CG1	2:D:625:LEU:N	2.60	0.64
2:D:120:CYS:O	2:D:134:ILE:HD12	1.99	0.63
2:D:641:ASN:O	2:D:641:ASN:ND2	2.30	0.63
2:D:653:TYR:O	2:D:654:LEU:HB3	1.99	0.63
2:B:192:ILE:HG12	2:B:375:ARG:HG2	1.80	0.63
1:A:312:LEU:HD12	1:A:315:PHE:HD1	1.63	0.63
2:B:626:ASP:CB	2:B:630:LYS:N	2.62	0.63
2:D:273:GLU:CG	2:D:306:ASP:OD1	2.46	0.63
2:B:562:ARG:N	2:B:563:GLN:HA	2.14	0.63
2:D:449:PRO:CD	2:D:455:MET:HE1	2.24	0.63
2:D:729:LYS:C	2:D:731:GLY:H	2.01	0.63
2:B:626:ASP:CB	2:B:630:LYS:H	2.12	0.62
2:D:113:GLU:HB3	2:D:114:PRO:CD	2.29	0.62
2:D:627:LEU:CD1	2:D:631:LEU:HD23	2.28	0.62
2:B:122:PHE:CD1	2:B:127:ILE:HD13	2.34	0.62
2:D:537:ILE:HD12	2:D:537:ILE:N	2.15	0.62
1:C:155:HIS:O	1:C:195:ARG:HD3	1.99	0.62
1:C:166:LEU:HD11	2:D:544:MET:HE1	1.81	0.62
1:C:66:GLN:HG2	1:C:67:VAL:H	1.64	0.62
1:C:58:ALA:HA	1:C:60:ILE:HD12	1.80	0.62
1:A:104:GLY:O	2:B:503:ASN:ND2	2.32	0.62
2:B:429:ILE:HG23	2:B:468:VAL:CG2	2.28	0.62
2:B:729:LYS:O	2:B:732:VAL:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ALA:HA	1:C:74:ARG:HG3	1.81	0.62
1:C:268:GLU:OE2	4:C:999:AMP:H3'	2.00	0.62
2:B:740:LEU:HD21	2:B:756:LEU:HB2	1.82	0.62
2:B:226:VAL:HG22	2:B:226:VAL:O	2.00	0.62
2:D:256:VAL:HG21	2:D:376:ALA:HB2	1.81	0.62
1:A:155:HIS:CG	1:A:168:THR:HG21	2.34	0.61
1:A:251:THR:O	1:A:252:GLU:HB2	2.00	0.61
2:B:672:LYS:O	2:B:673:LEU:HB2	2.00	0.61
2:B:272:ILE:CG1	2:B:273:GLU:N	2.63	0.61
2:D:26:THR:HG22	2:D:32:VAL:N	2.10	0.61
2:D:451:TRP:CD1	2:D:452:ARG:HG3	2.35	0.61
1:C:65:GLU:HA	1:C:66:GLN:C	2.20	0.61
2:D:786:LYS:HD2	2:D:791:ALA:CB	2.27	0.61
1:A:145:ILE:CG2	1:A:146:PRO:C	2.68	0.61
1:A:185:ILE:HD11	1:A:212:LEU:CD1	2.16	0.61
2:B:205:ILE:HG22	2:B:276:ILE:CB	2.30	0.61
2:D:56:HIS:HE1	2:D:58:ASN:HB3	1.55	0.61
2:D:111:ARG:C	2:D:113:GLU:H	2.03	0.61
2:D:253:THR:CG2	2:D:264:MET:HB2	2.28	0.61
1:A:205:MET:O	1:A:206:PHE:HB3	1.99	0.61
1:A:269:VAL:HG13	1:A:302:LEU:CD1	2.31	0.61
1:C:225:GLY:HA2	2:D:476:ASP:HB3	1.83	0.61
2:D:626:ASP:O	2:D:627:LEU:C	2.37	0.61
1:C:124:GLY:HA3	1:C:186:ARG:HH11	1.66	0.61
2:B:78:VAL:CG1	2:B:115:SER:HB3	2.28	0.61
2:B:427:THR:HG23	2:B:444:TRP:HE1	1.66	0.61
2:D:115:SER:C	2:D:116:GLU:O	2.38	0.61
2:D:452:ARG:HH11	2:D:452:ARG:CG	2.05	0.61
2:D:121:SER:HA	2:D:135:ILE:HG13	1.82	0.61
2:B:734:GLN:HG3	2:B:777:THR:HG21	1.83	0.61
2:B:68:ASN:ND2	2:B:143:ILE:HG21	2.15	0.60
2:B:271:ARG:HH21	2:B:321:HIS:HD2	1.47	0.60
2:B:31:GLU:HG2	2:B:161:SER:HB2	1.83	0.60
2:D:119:LEU:HB3	2:D:134:ILE:CD1	2.31	0.60
2:D:634:VAL:HG12	2:D:635:GLU:N	2.16	0.60
1:C:166:LEU:HD11	2:D:544:MET:CE	2.31	0.60
2:D:631:LEU:C	2:D:633:GLU:H	2.05	0.60
2:D:56:HIS:CG	2:D:57:PRO:HA	2.35	0.60
1:A:202:HIS:CE1	4:A:992:AMP:O2P	2.55	0.60
2:B:24:GLN:NE2	2:B:183:ASN:OD1	2.31	0.60
2:D:659:ILE:HD12	2:D:684:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:644:LEU:HD13	2:B:649:SER:CB	2.27	0.60
2:B:576:PHE:CD1	2:B:588:GLN:HG2	2.37	0.60
2:B:630:LYS:HB3	2:B:631:LEU:C	2.22	0.60
2:D:55:GLN:CA	2:D:56:HIS:O	2.48	0.60
2:D:56:HIS:CB	2:D:57:PRO:CA	2.72	0.60
2:B:269:LYS:O	2:B:272:ILE:HD12	2.01	0.60
1:C:242:ARG:HB2	1:C:257:VAL:O	2.01	0.60
2:D:499:LYS:CD	2:D:570:PHE:HE1	2.10	0.60
2:B:137:LEU:O	2:B:139:ALA:N	2.33	0.60
2:D:47:VAL:CG2	2:D:142:PRO:O	2.49	0.60
2:D:76:ASP:OD2	2:D:114:PRO:HB3	2.02	0.59
2:B:209:ALA:H	2:B:210:PRO:HD3	1.68	0.59
2:B:627:LEU:HD22	1:C:100:ARG:HH12	1.67	0.59
1:C:61:ASN:O	1:C:64:LYS:N	2.32	0.59
2:D:473:ASN:H	2:D:473:ASN:HD22	1.48	0.59
2:D:566:ARG:HG3	2:D:566:ARG:HH11	1.68	0.59
2:B:633:GLU:HB3	2:B:655:LYS:H	1.66	0.59
1:C:300:GLU:H	1:C:300:GLU:CD	2.05	0.59
2:D:643:ALA:HB1	2:D:669:LEU:CD2	2.33	0.59
1:A:140:PHE:HA	1:A:145:ILE:HG12	1.81	0.59
1:A:149:HIS:ND1	1:A:150:PRO:HD2	2.17	0.59
2:D:19:ASP:OD1	2:D:19:ASP:N	2.35	0.59
2:D:127:ILE:HG12	2:D:239:ARG:CZ	2.32	0.59
1:A:133:ILE:CD1	2:B:576:PHE:CD1	2.85	0.59
2:B:787:GLU:O	2:B:787:GLU:HG3	2.03	0.59
2:D:263:PRO:HB2	2:D:360:TYR:CE2	2.38	0.59
2:D:26:THR:CG2	2:D:32:VAL:H	2.12	0.59
2:D:205:ILE:HD11	2:D:392:ILE:HB	1.83	0.59
2:D:634:VAL:CG1	2:D:635:GLU:N	2.66	0.59
1:A:300:GLU:CB	1:A:312:LEU:CD1	2.79	0.59
2:B:257:LEU:HA	2:B:262:GLN:O	2.03	0.59
2:B:666:HIS:ND1	2:B:668:GLU:OE1	2.35	0.59
1:C:108:PRO:HG3	1:C:326:PHE:CD2	2.37	0.59
2:B:750:ALA:HB3	2:B:753:TYR:HD1	1.68	0.59
1:A:140:PHE:HD1	1:A:145:ILE:HG13	1.66	0.59
1:A:314:SER:HA	1:A:317:GLU:HG3	1.85	0.59
1:A:143:LEU:HD11	1:A:171:SER:HB3	1.84	0.58
2:D:49:GLU:HB3	2:D:89:ARG:HD3	1.85	0.58
2:D:689:LEU:O	2:D:689:LEU:HG	2.02	0.58
2:D:711:ALA:HB3	2:D:793:LEU:O	2.03	0.58
2:B:90:VAL:HG13	2:B:91:ALA:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLU:C	1:C:64:LYS:H	2.05	0.58
2:D:515:PHE:HA	2:D:543:ALA:O	2.03	0.58
1:A:107:HIS:CG	1:A:108:PRO:HD2	2.38	0.58
2:D:142:PRO:O	2:D:144:GLY:N	2.36	0.58
2:D:272:ILE:O	2:D:306:ASP:HB2	2.03	0.58
2:D:735:VAL:HA	2:D:762:LEU:HD23	1.86	0.58
1:C:62:GLU:C	1:C:64:LYS:N	2.57	0.58
1:C:218:ILE:HG12	1:C:222:ASN:HD22	1.67	0.58
2:D:32:VAL:HB	2:D:158:ILE:CD1	2.32	0.58
2:D:473:ASN:ND2	2:D:473:ASN:N	2.49	0.58
2:D:306:ASP:OD2	2:D:306:ASP:C	2.42	0.58
2:D:713:VAL:O	2:D:714:VAL:HG23	2.04	0.58
1:C:60:ILE:O	1:C:61:ASN:C	2.42	0.58
2:D:370:HIS:O	2:D:374:GLU:HG2	2.04	0.58
2:D:762:LEU:HD12	2:D:774:ILE:HG23	1.85	0.58
1:A:156:ASP:CB	1:A:196:ASN:HB3	2.34	0.58
2:B:629:GLY:HA2	2:B:692:ARG:HB2	1.85	0.58
2:B:652:ILE:HD11	2:B:662:VAL:HG22	1.85	0.58
1:C:17:GLN:C	1:C:19:SER:H	2.06	0.58
1:C:139:ASN:HD21	1:C:168:THR:H	1.51	0.58
2:B:111:ARG:HG3	2:B:111:ARG:HH11	1.69	0.58
1:C:65:GLU:O	1:C:65:GLU:HG2	2.04	0.58
1:A:107:HIS:HE1	1:A:315:PHE:O	1.87	0.58
1:A:166:LEU:CD1	2:B:544:MET:HE1	2.32	0.58
2:B:287:LEU:O	2:B:294:GLU:HA	2.04	0.57
2:B:698:ARG:H	1:C:325:GLN:HE22	1.50	0.57
2:B:644:LEU:HA	2:B:666:HIS:H	1.68	0.57
1:C:251:THR:OG1	1:C:254:SER:HB3	2.05	0.57
2:B:214:PRO:HD2	2:B:337:PHE:HD2	1.69	0.57
2:B:750:ALA:O	2:B:753:TYR:HB2	2.04	0.57
1:A:145:ILE:HG21	1:A:146:PRO:O	2.03	0.57
2:D:319:GLY:C	2:D:321:HIS:H	2.05	0.57
2:D:626:ASP:CB	2:D:627:LEU:HD12	2.35	0.57
2:B:621:LEU:O	2:B:625:LEU:N	2.31	0.57
1:C:258:ASP:HA	1:C:267:LEU:O	2.04	0.57
1:C:304:MET:HA	1:C:309:VAL:HB	1.85	0.57
2:D:732:VAL:CG1	2:D:733:ASN:H	2.09	0.57
1:A:202:HIS:HE1	4:A:992:AMP:O2P	1.86	0.57
2:B:195:VAL:HG21	2:B:377:THR:HG22	1.87	0.57
2:B:577:VAL:HG23	2:B:587:ARG:HB3	1.87	0.57
1:C:301:ARG:HD2	4:C:999:AMP:C2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:735:VAL:HB	2:D:762:LEU:HD23	1.87	0.57
2:B:767:ARG:HH11	2:B:767:ARG:HB3	1.68	0.57
1:C:253:PRO:HB3	2:D:463:GLU:HA	1.87	0.57
2:D:533:LEU:HD23	2:D:536:PRO:HB3	1.87	0.57
2:D:626:ASP:CB	2:D:631:LEU:CD2	2.82	0.57
1:A:203:THR:N	4:A:992:AMP:N6	2.52	0.56
2:B:436:GLU:HB3	2:B:447:VAL:HB	1.86	0.56
1:A:134:GLU:HB3	1:A:165:LEU:CD2	2.34	0.56
1:C:88:ALA:O	1:C:91:THR:HG23	2.04	0.56
1:C:277:PRO:HG3	2:D:459:GLU:CD	2.25	0.56
2:D:92:VAL:HG13	2:D:119:LEU:HD23	1.87	0.56
1:A:145:ILE:HG22	1:A:146:PRO:N	2.19	0.56
1:A:243:PHE:HD2	1:A:257:VAL:HG12	1.69	0.56
2:B:644:LEU:CD1	2:B:649:SER:HB2	2.32	0.56
1:C:257:VAL:HG23	1:C:269:VAL:HG23	1.86	0.56
2:D:115:SER:O	2:D:116:GLU:C	2.43	0.56
2:B:2:LYS:HB3	2:B:159:GLU:HB2	1.86	0.56
2:B:376:ALA:HA	2:B:379:LEU:HD22	1.86	0.56
2:D:38:VAL:HG11	2:D:240:ARG:HD3	1.88	0.56
1:A:136:ASP:OD1	1:A:152:ARG:CZ	2.54	0.56
2:B:50:VAL:HA	2:B:67:VAL:HG12	1.88	0.56
2:B:650:ALA:O	2:B:661:PHE:HD1	1.88	0.56
1:C:167:ARG:NH2	1:C:191:GLY:HA3	2.21	0.56
2:D:205:ILE:O	2:D:394:ILE:HD13	2.06	0.56
1:A:210:GLU:HA	1:A:295:PHE:O	2.06	0.56
2:B:256:VAL:HG13	2:B:260:LEU:HD12	1.87	0.56
2:B:626:ASP:C	2:B:629:GLY:H	2.09	0.56
2:D:555:THR:O	2:D:559:ASN:ND2	2.38	0.56
1:A:178:MET:SD	1:A:212:LEU:HD11	2.46	0.56
2:B:741:PHE:CB	2:D:603:GLU:HG3	2.36	0.56
1:A:139:ASN:ND2	1:A:168:THR:HB	2.09	0.56
1:A:156:ASP:HB3	1:A:196:ASN:HB3	1.87	0.56
2:D:7:TRP:O	2:D:10:GLU:HB2	2.06	0.56
2:B:283:GLU:HG2	2:B:299:ALA:HB2	1.88	0.56
2:B:477:GLU:OE1	2:B:478:PRO:HD2	2.06	0.56
2:B:575:ARG:O	2:B:588:GLN:HA	2.06	0.56
2:B:121:SER:OG	2:B:124:GLU:HG2	2.06	0.55
2:B:488:HIS:H	2:B:488:HIS:CD2	2.23	0.55
1:C:241:ILE:H	1:C:241:ILE:HD13	1.71	0.55
2:B:708:ARG:O	2:B:760:LEU:HD12	2.06	0.55
1:C:58:ALA:CA	1:C:60:ILE:HG21	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LEU:O	1:C:91:THR:CG2	2.54	0.55
1:A:252:GLU:OE2	2:B:463:GLU:CD	2.45	0.55
2:B:562:ARG:H	2:B:563:GLN:HA	1.71	0.55
2:B:576:PHE:CE1	2:B:588:GLN:HG2	2.41	0.55
1:C:62:GLU:O	1:C:65:GLU:N	2.35	0.55
2:D:280:MET:HG2	2:D:299:ALA:O	2.07	0.55
2:B:202:THR:CG2	2:B:392:ILE:HD11	2.36	0.55
2:D:470:GLY:HA3	2:D:473:ASN:HD21	1.71	0.55
2:B:783:GLU:HA	2:B:786:LYS:HB2	1.88	0.55
1:C:228:HIS:HB2	1:C:243:PHE:HZ	1.70	0.55
2:D:338:PHE:CD2	2:D:360:TYR:CE1	2.94	0.55
2:D:553:LEU:HA	2:D:556:VAL:CG1	2.37	0.55
2:B:127:ILE:HG13	2:B:239:ARG:CZ	2.37	0.55
2:B:209:ALA:N	2:B:210:PRO:HD3	2.22	0.55
2:D:408:LEU:HD23	2:D:458:GLU:HG3	1.89	0.55
1:A:158:PHE:CD2	1:A:195:ARG:O	2.54	0.55
2:B:53:CYS:SG	2:B:63:ARG:HG2	2.47	0.55
2:D:729:LYS:NZ	2:D:729:LYS:HB3	2.21	0.55
2:B:139:ALA:C	2:B:141:ALA:N	2.59	0.55
2:B:483:LEU:HB3	1:C:123:LEU:HG	1.88	0.55
1:C:301:ARG:CD	4:C:999:AMP:C2	2.89	0.55
2:D:375:ARG:CG	2:D:375:ARG:NH1	2.47	0.55
2:B:631:LEU:CD2	2:B:632:ASN:H	2.20	0.54
2:D:617:LEU:HD23	2:D:662:VAL:HG23	1.89	0.54
1:C:171:SER:HA	1:C:210:GLU:CD	2.28	0.54
2:D:723:ILE:HG23	2:D:785:LEU:HD22	1.89	0.54
2:D:764:ASP:OD2	2:D:765:THR:N	2.40	0.54
1:A:218:ILE:HD12	1:A:219:SER:N	2.22	0.54
2:B:294:GLU:CD	2:B:294:GLU:H	2.10	0.54
2:B:641:ASN:O	2:B:643:ALA:N	2.40	0.54
2:B:134:ILE:HD12	2:B:134:ILE:N	2.23	0.54
2:B:524:ILE:O	2:B:643:ALA:HB2	2.07	0.54
2:B:662:VAL:HG13	2:B:682:PHE:HB3	1.89	0.54
1:C:58:ALA:HB1	1:C:61:ASN:N	2.23	0.54
2:D:606:ASN:CG	2:D:606:ASN:O	2.46	0.54
2:D:698:ARG:O	2:D:699:GLU:O	2.26	0.54
2:B:7:TRP:HD1	2:B:7:TRP:O	1.91	0.54
2:B:7:TRP:O	2:B:7:TRP:CD1	2.61	0.54
2:B:59:ALA:HB2	2:B:111:ARG:HG2	1.89	0.54
2:B:256:VAL:HG21	2:B:376:ALA:HB2	1.90	0.54
2:B:272:ILE:O	2:B:273:GLU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:641:ASN:HB2	2:D:661:PHE:CE1	2.41	0.54
2:D:733:ASN:HA	2:D:734:GLN:CB	2.30	0.54
2:B:522:GLN:O	2:B:526:PRO:HA	2.07	0.54
2:B:724:LEU:HD12	2:B:738:VAL:HB	1.90	0.54
1:C:140:PHE:HD1	1:C:145:ILE:HD13	1.72	0.54
1:C:220:PHE:O	1:C:223:LEU:N	2.40	0.54
2:D:76:ASP:OD2	2:D:114:PRO:CB	2.56	0.54
1:A:192:ARG:NH2	2:B:512:THR:O	2.41	0.54
2:B:521:GLN:NE2	2:B:546:LEU:H	2.06	0.54
1:C:21:VAL:HA	1:C:24:LEU:HB2	1.90	0.54
2:B:641:ASN:C	2:B:643:ALA:H	2.10	0.54
2:D:127:ILE:C	2:D:127:ILE:CD1	2.76	0.54
1:A:160:PHE:CE1	1:A:166:LEU:HG	2.43	0.54
2:D:560:GLN:HG2	2:D:675:LEU:HB3	1.89	0.54
2:B:338:PHE:CB	2:B:343:ILE:HD11	2.39	0.53
2:B:457:ILE:HG22	2:B:460:ASP:CG	2.27	0.53
2:B:517:ASP:CA	2:B:540:GLU:O	2.56	0.53
2:B:647:GLY:HA3	1:C:91:THR:HB	1.90	0.53
1:C:257:VAL:CG2	1:C:269:VAL:HG23	2.38	0.53
2:D:55:GLN:CG	2:D:56:HIS:HA	2.36	0.53
2:D:109:LYS:HA	2:D:115:SER:HA	1.90	0.53
1:A:151:ALA:O	1:A:154:ASP:N	2.41	0.53
1:A:164:ARG:NH1	2:B:585:GLY:N	2.42	0.53
2:B:304:ILE:O	2:B:311:LEU:HD22	2.09	0.53
2:B:630:LYS:HB3	2:B:631:LEU:CA	2.38	0.53
2:B:674:ASP:O	2:B:675:LEU:CB	2.55	0.53
2:D:205:ILE:CG2	2:D:276:ILE:HB	2.36	0.53
1:C:58:ALA:HA	1:C:60:ILE:HG21	1.89	0.53
1:A:218:ILE:CD1	1:A:293:PHE:CD1	2.92	0.53
1:A:270:LEU:C	1:A:270:LEU:HD12	2.29	0.53
2:D:630:LYS:NZ	2:D:691:ASP:OD2	2.42	0.53
1:A:312:LEU:HD12	1:A:315:PHE:CD1	2.44	0.53
2:B:370:HIS:CE1	2:B:393:ASP:OD1	2.62	0.53
1:C:82:ALA:O	1:C:85:ALA:N	2.41	0.53
2:B:565:ASN:OD1	2:B:566:ARG:N	2.34	0.53
2:D:312:ALA:HB1	2:D:317:PHE:O	2.09	0.53
2:D:729:LYS:C	2:D:731:GLY:N	2.63	0.53
1:C:5:ALA:O	1:C:9:ALA:HB3	2.09	0.53
2:D:57:PRO:CB	2:D:59:ALA:O	2.57	0.53
2:D:498:VAL:HG13	2:D:624:VAL:HG13	1.90	0.53
2:B:45:VAL:HG13	2:B:92:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:HIS:ND1	1:C:301:ARG:NH2	2.56	0.53
2:B:32:VAL:HG12	2:B:160:ILE:HG22	1.91	0.52
2:B:376:ALA:HA	2:B:379:LEU:CD2	2.40	0.52
1:C:71:LEU:C	1:C:73:ALA:H	2.13	0.52
2:D:549:TRP:O	2:D:553:LEU:HG	2.10	0.52
2:D:634:VAL:HG23	2:D:654:LEU:HD13	1.91	0.52
1:A:185:ILE:CG1	1:A:186:ARG:N	2.72	0.52
1:A:244:ARG:NH1	1:A:256:GLU:OE2	2.42	0.52
1:C:218:ILE:HG23	1:C:218:ILE:O	2.09	0.52
2:D:263:PRO:HB2	2:D:360:TYR:HE2	1.74	0.52
2:D:653:TYR:O	2:D:654:LEU:CB	2.57	0.52
1:A:86:ARG:HG2	1:A:90:GLU:OE1	2.08	0.52
2:B:4:SER:HB3	2:B:7:TRP:HB2	1.91	0.52
2:B:165:ASN:H	2:B:165:ASN:ND2	2.01	0.52
1:C:56:ALA:N	1:C:57:GLY:HA3	2.24	0.52
1:C:194:TYR:OH	2:D:514:SER:HB2	2.09	0.52
2:D:199:ILE:HD13	2:D:222:LYS:HG2	1.90	0.52
2:D:358:HIS:O	2:D:362:ARG:HD3	2.08	0.52
1:A:145:ILE:HG22	1:A:146:PRO:CA	2.39	0.52
2:B:123:SER:O	2:B:125:LEU:N	2.42	0.52
2:B:603:GLU:OE1	2:B:603:GLU:HA	2.10	0.52
2:B:739:ASN:ND2	2:B:740:LEU:H	2.08	0.52
1:C:190:PRO:N	1:C:209:MET:HE3	2.25	0.52
1:C:211:GLY:HA3	1:C:295:PHE:CZ	2.44	0.52
2:D:624:VAL:O	2:D:625:LEU:C	2.46	0.52
2:D:735:VAL:HB	2:D:762:LEU:CD2	2.39	0.52
1:C:58:ALA:HA	1:C:60:ILE:HB	1.79	0.52
1:C:255:ALA:HB2	2:D:471:TYR:HE2	1.75	0.52
1:A:247:TYR:CE1	2:B:165:ASN:HB3	2.45	0.52
2:D:672:LYS:O	2:D:674:ASP:CB	2.58	0.52
2:D:631:LEU:CG	2:D:632:ASN:H	2.21	0.52
1:A:201:THR:C	1:A:312:LEU:HD23	2.29	0.52
1:A:218:ILE:CD1	1:A:293:PHE:HD1	2.23	0.52
2:B:205:ILE:O	2:B:394:ILE:HD13	2.10	0.52
2:B:344:THR:HA	2:B:361:GLU:CD	2.31	0.52
2:B:521:GLN:HE22	2:B:545:ARG:HA	1.74	0.52
1:C:241:ILE:H	1:C:241:ILE:CD1	2.22	0.52
2:D:548:LEU:HD23	2:D:571:GLU:HB3	1.91	0.52
2:D:731:GLY:HA2	2:D:735:VAL:HG13	1.92	0.52
1:C:59:VAL:O	1:C:59:VAL:CG1	2.53	0.51
1:C:322:PHE:O	1:C:325:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:HIS:O	2:D:97:ALA:HB1	2.09	0.51
2:D:288:VAL:HA	2:D:294:GLU:HA	1.91	0.51
2:D:702:ARG:NE	2:D:702:ARG:N	2.55	0.51
1:A:86:ARG:O	1:A:90:GLU:HB2	2.10	0.51
1:A:318:ASN:HD22	1:A:323:LEU:HD21	1.74	0.51
2:B:38:VAL:HB	2:B:155:ASP:O	2.09	0.51
2:B:264:MET:CE	2:B:376:ALA:HB2	2.41	0.51
2:B:626:ASP:C	2:B:628:THR:N	2.62	0.51
1:C:257:VAL:O	1:C:258:ASP:HB2	2.10	0.51
1:A:269:VAL:HG13	1:A:302:LEU:HD13	1.91	0.51
2:B:264:MET:HE1	2:B:376:ALA:HB2	1.91	0.51
1:C:23:ALA:HA	1:C:74:ARG:CG	2.40	0.51
1:C:132:GLU:HA	1:C:167:ARG:HD3	1.92	0.51
1:C:185:ILE:HD13	1:C:185:ILE:C	2.30	0.51
2:D:24:GLN:HG3	2:D:182:LEU:HD22	1.92	0.51
2:D:142:PRO:C	2:D:144:GLY:H	2.13	0.51
1:A:218:ILE:HD13	1:A:293:PHE:HD1	1.74	0.51
2:B:17:ASP:OD1	2:B:18:SER:N	2.44	0.51
2:B:630:LYS:CB	2:B:631:LEU:O	2.50	0.51
2:B:631:LEU:HD23	2:B:632:ASN:N	2.26	0.51
1:C:211:GLY:HA3	1:C:295:PHE:CE2	2.45	0.51
2:D:55:GLN:C	2:D:56:HIS:O	2.48	0.51
2:D:593:ALA:HB2	2:D:683:GLU:HG3	1.91	0.51
2:D:709:ASP:HA	2:D:759:SER:HA	1.91	0.51
1:A:270:LEU:CB	1:A:297:MET:HB3	2.38	0.51
1:C:119:PHE:CD1	1:C:119:PHE:N	2.78	0.51
2:B:48:GLY:HA2	2:B:143:ILE:HG23	1.93	0.51
2:B:55:GLN:C	2:B:56:HIS:CG	2.84	0.51
2:B:501:LEU:HA	2:D:504:ASP:OD2	2.11	0.51
2:B:517:ASP:HA	2:B:540:GLU:O	2.10	0.51
2:B:90:VAL:O	2:B:137:LEU:HD22	2.11	0.51
2:B:790:GLN:CG	2:B:791:ALA:H	2.24	0.51
2:D:183:ASN:HB2	2:D:185:LEU:HD12	1.91	0.51
2:D:452:ARG:HG2	2:D:452:ARG:NH1	1.97	0.51
2:B:613:ASP:OD2	2:B:613:ASP:C	2.49	0.51
2:D:137:LEU:HB3	2:D:138:PRO:HD2	1.92	0.51
1:A:118:SER:O	1:A:119:PHE:C	2.49	0.50
2:B:38:VAL:HG21	2:B:240:ARG:CD	2.40	0.50
2:D:605:TRP:CE3	2:D:606:ASN:HB2	2.45	0.50
1:A:86:ARG:HG2	1:A:90:GLU:CD	2.31	0.50
2:B:232:LEU:O	2:B:235:LYS:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:744:TYR:OH	2:B:747:LYS:N	2.44	0.50
1:C:132:GLU:CD	2:D:574:LEU:HD11	2.31	0.50
2:D:731:GLY:HA2	2:D:735:VAL:CG1	2.41	0.50
2:B:614:PHE:CZ	1:C:94:VAL:HG22	2.46	0.50
2:D:441:LYS:HG2	2:D:441:LYS:O	2.09	0.50
2:B:520:VAL:O	2:B:523:MET:HB2	2.11	0.50
2:D:85:ARG:HB3	2:D:88:LEU:HD11	1.91	0.50
2:D:672:LYS:O	2:D:674:ASP:CG	2.49	0.50
1:A:185:ILE:O	1:A:186:ARG:HB2	2.11	0.50
1:A:243:PHE:CD2	1:A:257:VAL:HG12	2.46	0.50
1:A:300:GLU:CB	1:A:312:LEU:HD11	2.41	0.50
2:B:177:ARG:HA	2:B:187:LEU:HD13	1.93	0.50
2:D:137:LEU:HB3	2:D:138:PRO:CD	2.42	0.50
2:B:138:PRO:O	2:B:139:ALA:O	2.30	0.50
1:C:211:GLY:O	1:C:294:ALA:HA	2.11	0.50
2:D:41:SER:HA	2:D:148:ARG:HH21	1.77	0.50
2:B:525:HIS:HE1	2:B:547:SER:OG	1.94	0.50
2:D:54:ALA:O	2:D:55:GLN:O	2.29	0.50
2:D:670:GLU:OE2	2:D:671:ARG:NH2	2.44	0.50
1:A:97:PRO:HD2	2:B:605:TRP:CD1	2.47	0.50
2:B:687:ASN:OD1	2:B:687:ASN:C	2.49	0.50
2:D:53:CYS:O	2:D:54:ALA:O	2.30	0.50
2:D:346:ARG:N	2:D:346:ARG:HD2	2.27	0.50
2:B:698:ARG:H	1:C:325:GLN:NE2	2.10	0.50
1:C:58:ALA:HA	1:C:60:ILE:CG2	2.39	0.50
1:C:149:HIS:O	1:C:150:PRO:C	2.50	0.50
1:A:268:GLU:HB3	1:A:301:ARG:HH21	1.78	0.49
2:B:37:PRO:HA	2:B:156:ASN:HD22	1.75	0.49
2:B:122:PHE:CD1	2:B:127:ILE:CD1	2.95	0.49
2:B:591:MET:HE3	2:B:684:LEU:O	2.11	0.49
2:B:741:PHE:HB3	2:D:603:GLU:HG3	1.94	0.49
1:C:251:THR:HB	1:C:273:GLY:HA3	1.93	0.49
2:D:515:PHE:CD1	2:D:544:MET:HE1	2.37	0.49
1:C:50:PRO:O	1:C:52:GLU:N	2.45	0.49
2:D:17:ASP:HB3	2:D:20:ALA:H	1.76	0.49
2:D:279:ARG:NH1	2:D:280:MET:O	2.45	0.49
2:D:547:SER:OG	2:D:549:TRP:HB2	2.12	0.49
2:B:123:SER:C	2:B:125:LEU:H	2.15	0.49
1:C:69:GLN:HE21	1:C:69:GLN:CA	2.23	0.49
1:C:265:LYS:NZ	2:D:33:ASP:HB2	2.27	0.49
1:C:265:LYS:HD2	1:C:266:TRP:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ASN:O	2:B:134:ILE:HD11	2.12	0.49
2:B:90:VAL:CG1	2:B:91:ALA:N	2.75	0.49
2:B:204:PRO:HD2	2:B:275:GLY:HA2	1.94	0.49
1:A:195:ARG:HD2	1:A:206:PHE:HE1	1.77	0.49
2:B:208:GLU:O	2:B:209:ALA:HB2	2.13	0.49
2:B:271:ARG:HH21	2:B:321:HIS:CD2	2.29	0.49
2:B:615:TYR:HB2	1:C:99:ARG:NH1	2.28	0.49
1:A:143:LEU:O	1:A:250:PHE:HB3	2.12	0.49
2:B:181:VAL:HG11	2:B:433:LEU:HD13	1.94	0.49
2:B:653:TYR:O	2:B:657:GLU:O	2.30	0.49
1:C:174:GLN:OE1	1:C:210:GLU:OE2	2.30	0.49
2:D:54:ALA:HB3	2:D:64:VAL:HG13	1.94	0.49
2:D:668:GLU:HG2	2:D:672:LYS:HE3	1.93	0.49
1:A:189:ALA:HB3	1:A:210:GLU:HB2	1.94	0.49
1:C:105:GLY:HA3	2:D:508:GLN:OE1	2.12	0.49
2:B:338:PHE:HB3	2:B:343:ILE:HD11	1.94	0.49
2:B:515:PHE:HD1	2:B:544:MET:CE	2.24	0.49
2:B:583:PRO:C	2:B:584:LEU:O	2.51	0.49
2:B:625:LEU:C	2:B:627:LEU:H	2.09	0.49
2:B:794:ARG:HA	2:B:795:ASP:C	2.34	0.49
1:C:45:LEU:CB	1:C:46:ARG:HA	2.42	0.49
1:C:54:PRO:N	1:C:55:ALA:CA	2.70	0.49
1:C:202:HIS:HA	4:C:999:AMP:HN61	1.76	0.49
1:C:216:THR:O	1:C:217:ASN:O	2.30	0.49
2:D:630:LYS:NZ	2:D:691:ASP:O	2.35	0.49
2:D:548:LEU:HD12	2:D:548:LEU:N	2.28	0.49
2:B:111:ARG:HH11	2:B:111:ARG:CG	2.26	0.49
2:B:280:MET:HG3	2:B:299:ALA:O	2.13	0.49
1:C:242:ARG:O	1:C:257:VAL:HA	2.12	0.49
2:D:113:GLU:O	2:D:114:PRO:O	2.30	0.49
2:D:713:VAL:H	2:D:792:SER:HA	1.78	0.49
2:B:710:ILE:HD11	2:B:758:ILE:HB	1.95	0.48
2:D:493:LEU:HB2	2:D:692:ARG:HD3	1.94	0.48
2:B:309:LYS:NZ	2:B:321:HIS:CE1	2.81	0.48
1:C:244:ARG:O	1:C:255:ALA:HB1	2.14	0.48
2:D:556:VAL:HG23	2:D:560:GLN:OE1	2.12	0.48
2:D:570:PHE:HA	2:D:593:ALA:O	2.13	0.48
2:D:634:VAL:HG22	2:D:654:LEU:CB	2.34	0.48
1:A:99:ARG:HB3	2:B:607:LEU:HD21	1.95	0.48
1:A:182:GLN:HG3	1:A:183:PRO:HD2	1.95	0.48
1:A:230:PHE:HB2	2:D:485:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:GLN:NE2	2:B:529:GLU:CD	2.66	0.48
1:C:59:VAL:H	1:C:60:ILE:CB	2.23	0.48
2:D:55:GLN:HG3	2:D:56:HIS:HA	1.95	0.48
2:D:631:LEU:O	2:D:633:GLU:N	2.45	0.48
1:A:107:HIS:NE2	1:A:109:VAL:HG13	2.29	0.48
1:A:170:THR:C	1:A:210:GLU:HG3	2.24	0.48
2:B:644:LEU:HA	2:B:666:HIS:N	2.28	0.48
1:C:66:GLN:O	1:C:67:VAL:HG22	2.13	0.48
1:C:235:PHE:HA	1:C:306:ARG:NH1	2.29	0.48
1:C:239:LEU:HD13	1:C:241:ILE:HD12	1.96	0.48
1:C:277:PRO:HG3	2:D:459:GLU:OE1	2.13	0.48
2:D:7:TRP:CD2	2:D:172:ILE:HD12	2.48	0.48
2:B:236:GLU:HG3	2:B:240:ARG:HE	1.79	0.48
2:B:252:VAL:HG21	2:B:380:LEU:HD13	1.95	0.48
2:B:631:LEU:CD2	2:B:632:ASN:N	2.77	0.48
2:D:30:LEU:N	2:D:30:LEU:HD23	2.29	0.48
2:D:664:VAL:HB	2:D:680:LEU:HD13	1.96	0.48
2:B:131:HIS:O	2:B:132:SER:HB2	2.14	0.48
2:B:432:ARG:CG	2:B:432:ARG:NH1	2.72	0.48
2:B:517:ASP:OD1	2:B:519:LYS:N	2.45	0.48
1:C:164:ARG:HH12	2:D:531:LEU:HD11	1.78	0.48
2:D:57:PRO:HG3	2:D:63:ARG:HH22	1.78	0.48
2:D:402:LYS:HB2	2:D:403:ARG:NH2	2.29	0.48
2:B:230:THR:HG23	2:B:234:MET:HE2	1.96	0.48
2:B:600:ARG:HH12	2:B:616:ASP:CG	2.12	0.48
2:B:666:HIS:CE1	2:B:668:GLU:OE2	2.67	0.48
2:D:234:MET:O	2:D:238:LEU:HB2	2.14	0.48
2:D:672:LYS:O	2:D:674:ASP:N	2.47	0.48
1:A:248:PHE:HD2	1:A:254:SER:HB3	1.79	0.48
1:A:289:VAL:HG12	1:A:290:TYR:CD1	2.48	0.48
2:D:11:TRP:CZ3	2:D:173:ILE:HG13	2.48	0.48
2:D:634:VAL:HA	2:D:654:LEU:HA	1.96	0.48
2:D:762:LEU:CD1	2:D:774:ILE:HG23	2.43	0.48
1:A:107:HIS:HD2	1:A:109:VAL:H	1.59	0.48
1:A:145:ILE:CG2	1:A:146:PRO:CA	2.91	0.48
1:A:174:GLN:HG3	1:A:212:LEU:HG	1.96	0.48
2:B:410:ARG:HH22	2:B:421:ILE:C	2.17	0.48
1:C:32:LEU:HA	1:C:35:LYS:HD3	1.96	0.48
1:C:140:PHE:CE2	1:C:165:LEU:HD11	2.48	0.48
1:C:279:VAL:O	1:C:282:ASN:HB2	2.14	0.48
2:D:306:ASP:HB3	2:D:311:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:ARG:HH21	2:B:464:GLU:CD	2.17	0.48
2:B:703:PHE:O	2:B:763:GLN:NE2	2.47	0.48
2:B:778:VAL:C	2:B:780:LYS:H	2.17	0.48
1:C:205:MET:HE2	2:D:513:TYR:HA	1.95	0.48
2:D:338:PHE:HD2	2:D:360:TYR:CD1	2.32	0.48
1:A:146:PRO:HG2	1:A:147:GLY:H	1.80	0.47
1:A:195:ARG:HB3	1:A:196:ASN:H	1.56	0.47
1:A:203:THR:N	4:A:992:AMP:HN61	2.00	0.47
1:A:313:ARG:NH1	1:A:317:GLU:OE1	2.47	0.47
1:C:284:GLY:C	1:C:285:ILE:HD12	2.35	0.47
1:C:324:LYS:HZ2	1:C:325:GLN:HB3	1.79	0.47
1:A:107:HIS:HD2	1:A:109:VAL:N	2.12	0.47
1:A:269:VAL:HG13	1:A:302:LEU:HD11	1.95	0.47
2:B:599:ASN:HA	2:B:611:THR:HA	1.95	0.47
1:C:265:LYS:HD2	1:C:266:TRP:H	1.80	0.47
2:D:55:GLN:O	2:D:63:ARG:HD3	2.14	0.47
1:A:169:GLN:CA	1:A:193:VAL:HG11	2.43	0.47
2:B:425:GLN:NE2	2:B:469:TYR:CD1	2.82	0.47
2:D:9:ARG:HA	2:D:12:VAL:O	2.14	0.47
2:D:42:PHE:CE2	2:D:125:LEU:HD22	2.49	0.47
2:D:571:GLU:N	2:D:593:ALA:O	2.44	0.47
1:A:199:ASP:OD1	1:A:202:HIS:HD2	1.97	0.47
1:C:238:ASP:CG	1:C:238:ASP:O	2.53	0.47
2:D:127:ILE:HD13	2:D:127:ILE:O	2.13	0.47
2:B:236:GLU:OE2	2:B:236:GLU:HA	2.15	0.47
2:B:306:ASP:OD1	2:B:308:ASN:HB3	2.14	0.47
2:D:111:ARG:C	2:D:113:GLU:N	2.68	0.47
2:D:184:GLN:HA	2:D:432:ARG:NH1	2.29	0.47
2:B:134:ILE:HD12	2:B:134:ILE:H	1.80	0.47
2:B:316:ILE:HD11	2:B:343:ILE:HG23	1.96	0.47
2:B:498:VAL:HG13	2:B:624:VAL:HG13	1.96	0.47
2:B:647:GLY:HA2	1:C:91:THR:HB	1.97	0.47
2:B:769:LEU:HD22	2:B:769:LEU:H	1.79	0.47
1:C:192:ARG:NH2	2:D:511:ILE:HG23	2.29	0.47
2:D:99:LEU:O	2:D:102:ASP:HA	2.15	0.47
2:D:133:GLY:O	2:D:134:ILE:HG22	2.14	0.47
2:D:139:ALA:O	2:D:141:ALA:N	2.48	0.47
2:D:165:ASN:O	2:D:166:ARG:C	2.53	0.47
2:D:605:TRP:CZ3	2:D:606:ASN:HB2	2.50	0.47
2:D:705:ALA:HB2	2:D:763:GLN:CD	2.35	0.47
1:A:185:ILE:HG13	1:A:186:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HA	1:A:297:MET:HA	1.96	0.47
2:B:659:ILE:HD11	2:B:688:LYS:HD3	1.95	0.47
1:C:268:GLU:CD	4:C:999:AMP:H3'	2.34	0.47
2:D:452:ARG:CG	2:D:452:ARG:NH1	2.72	0.47
2:D:621:LEU:O	2:D:625:LEU:HB3	2.14	0.47
2:D:671:ARG:HA	2:D:671:ARG:HD3	1.57	0.47
1:A:178:MET:CE	1:A:280:LEU:CD2	2.92	0.47
2:B:47:VAL:HG23	2:B:137:LEU:HD23	1.97	0.47
2:B:194:PRO:HA	2:B:374:GLU:CG	2.45	0.47
2:B:311:LEU:O	2:B:319:GLY:CA	2.62	0.47
2:B:427:THR:O	2:B:431:ARG:HB2	2.15	0.47
2:D:54:ALA:O	2:D:55:GLN:C	2.53	0.47
2:D:217:LEU:HB2	2:D:335:CYS:O	2.15	0.47
2:D:289:LEU:O	2:D:291:ASP:N	2.48	0.47
2:D:319:GLY:C	2:D:321:HIS:N	2.64	0.47
2:D:632:ASN:OD1	2:D:632:ASN:C	2.52	0.47
1:A:276:HIS:CD2	1:A:278:ASN:HB2	2.50	0.47
2:B:140:ASP:O	2:B:140:ASP:CG	2.53	0.47
2:B:165:ASN:N	2:B:165:ASN:ND2	2.60	0.47
2:B:194:PRO:HA	2:B:374:GLU:HG3	1.97	0.47
2:B:429:ILE:O	2:B:433:LEU:HD22	2.15	0.47
2:B:502:LEU:HD12	2:B:502:LEU:HA	1.80	0.47
2:D:38:VAL:HG13	2:D:155:ASP:O	2.15	0.47
1:A:140:PHE:CA	1:A:145:ILE:CG1	2.88	0.46
1:A:144:ASN:HB2	1:A:279:VAL:HG22	1.96	0.46
2:B:178:ASP:OD1	2:B:467:ARG:NH1	2.45	0.46
2:B:231:PRO:O	2:B:233:TRP:N	2.48	0.46
1:C:86:ARG:HG2	1:C:90:GLU:OE1	2.15	0.46
1:A:107:HIS:CD2	1:A:108:PRO:HD2	2.50	0.46
1:A:151:ALA:O	1:A:152:ARG:C	2.53	0.46
2:B:749:VAL:HG21	2:B:755:SER:HB2	1.97	0.46
2:B:767:ARG:NH1	2:B:767:ARG:CB	2.79	0.46
1:C:83:LEU:HD13	1:C:83:LEU:O	2.16	0.46
1:C:112:THR:HG1	1:C:234:PHE:HZ	1.63	0.46
1:C:196:ASN:OD1	2:D:537:ILE:HG23	2.16	0.46
2:D:271:ARG:HD3	2:D:321:HIS:CE1	2.49	0.46
2:D:669:LEU:HA	2:D:672:LYS:HD2	1.97	0.46
1:A:86:ARG:HG2	1:A:90:GLU:OE2	2.16	0.46
2:B:230:THR:HG22	2:B:235:LYS:HB2	1.96	0.46
2:D:107:ALA:HA	2:D:116:GLU:HB3	1.98	0.46
1:A:261:GLY:O	1:A:262:LYS:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:O	1:C:49:PRO:C	2.53	0.46
1:C:69:GLN:HA	1:C:69:GLN:NE2	2.26	0.46
2:D:17:ASP:HB2	2:D:20:ALA:HB2	1.96	0.46
2:D:201:ASP:OD1	2:D:201:ASP:N	2.48	0.46
2:D:699:GLU:OE1	2:D:699:GLU:CA	2.62	0.46
1:C:172:GLY:O	1:C:176:ARG:HG3	2.15	0.46
1:C:202:HIS:HE1	1:C:301:ARG:HH22	1.54	0.46
2:D:278:VAL:HG13	2:D:302:LEU:HD21	1.96	0.46
2:B:501:LEU:O	2:B:505:LYS:HG2	2.16	0.46
2:D:109:LYS:HB3	2:D:113:GLU:O	2.16	0.46
2:D:127:ILE:CD1	2:D:127:ILE:O	2.63	0.46
2:D:546:LEU:HD12	2:D:546:LEU:H	1.79	0.46
1:A:244:ARG:HD3	1:A:258:ASP:OD1	2.16	0.46
2:B:224:ILE:HG13	2:B:329:GLN:O	2.16	0.46
1:C:235:PHE:HA	1:C:306:ARG:HH11	1.81	0.46
2:D:65:THR:HG23	2:D:77:ILE:O	2.16	0.46
2:D:203:LEU:HD21	2:D:269:LYS:HE3	1.97	0.46
2:D:346:ARG:HD2	2:D:346:ARG:H	1.80	0.46
1:A:205:MET:O	1:A:206:PHE:CB	2.62	0.46
1:A:213:ILE:O	1:A:292:GLY:HA2	2.15	0.46
1:C:58:ALA:HB1	1:C:60:ILE:CB	2.40	0.46
2:D:666:HIS:ND1	2:D:668:GLU:OE1	2.49	0.46
1:A:98:GLY:HA2	2:D:615:TYR:HB3	1.98	0.46
1:A:108:PRO:HB2	1:A:303:THR:HG21	1.97	0.46
2:B:568:ARG:HB2	2:B:596:ILE:HG22	1.97	0.46
2:B:575:ARG:HG2	2:B:591:MET:SD	2.55	0.46
1:C:83:LEU:O	1:C:87:LEU:HG	2.14	0.46
1:A:279:VAL:CA	1:A:282:ASN:HD21	2.12	0.46
2:B:230:THR:HA	2:B:231:PRO:HD3	1.87	0.46
2:B:630:LYS:CB	2:B:631:LEU:CA	2.93	0.46
2:B:678:ARG:HD2	2:B:680:LEU:HD11	1.97	0.46
1:C:107:HIS:ND1	1:C:107:HIS:C	2.69	0.46
1:C:136:ASP:OD1	1:C:152:ARG:NH2	2.49	0.46
1:C:147:GLY:HA2	1:C:152:ARG:CZ	2.46	0.46
1:C:301:ARG:NE	4:C:999:AMP:C2	2.84	0.46
2:D:507:TYR:HB3	2:D:570:PHE:HD2	1.80	0.46
2:B:47:VAL:HG13	2:B:144:GLY:H	1.81	0.45
2:B:409:ARG:O	2:B:410:ARG:C	2.54	0.45
1:A:257:VAL:HG22	1:A:270:LEU:HG	1.98	0.45
2:B:111:ARG:N	2:B:112:GLY:CA	2.71	0.45
2:B:127:ILE:HG13	2:B:239:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:ASN:O	2:B:184:GLN:HG2	2.17	0.45
2:B:73:ARG:HG3	2:B:73:ARG:HH11	1.81	0.45
2:B:276:ILE:HG22	2:B:276:ILE:O	2.16	0.45
2:B:701:SER:HB2	2:B:703:PHE:HB2	1.99	0.45
1:C:320:LEU:HD13	1:C:320:LEU:HA	1.56	0.45
2:D:264:MET:SD	2:D:335:CYS:HB2	2.55	0.45
1:A:119:PHE:CD1	1:A:119:PHE:N	2.82	0.45
1:A:251:THR:HA	1:A:274:MET:O	2.16	0.45
1:C:241:ILE:CD1	1:C:241:ILE:N	2.79	0.45
2:B:521:GLN:HE22	2:B:546:LEU:H	1.64	0.45
2:B:522:GLN:HE22	2:B:529:GLU:CD	2.17	0.45
2:B:672:LYS:O	2:B:673:LEU:CB	2.65	0.45
1:C:111:ARG:O	1:C:115:ARG:HB2	2.17	0.45
2:D:257:LEU:HA	2:D:262:GLN:O	2.16	0.45
1:A:222:ASN:HA	2:B:477:GLU:O	2.17	0.45
1:C:192:ARG:CG	1:C:207:HIS:CE1	2.99	0.45
2:D:635:GLU:HG2	2:D:653:TYR:HB2	1.99	0.45
2:B:231:PRO:CG	2:B:383:ILE:HG12	2.47	0.45
2:D:199:ILE:HG12	2:D:388:ALA:O	2.17	0.45
2:B:56:HIS:HB2	2:B:59:ALA:O	2.17	0.45
2:B:110:LEU:O	2:B:111:ARG:CB	2.65	0.45
1:C:58:ALA:HA	1:C:60:ILE:CD1	2.45	0.45
1:C:64:LYS:O	1:C:65:GLU:HB3	2.17	0.45
2:D:631:LEU:C	2:D:633:GLU:N	2.70	0.45
2:D:644:LEU:HD13	2:D:649:SER:CB	2.40	0.45
1:A:176:ARG:NH2	1:A:176:ARG:HG3	2.32	0.45
1:A:190:PRO:HA	1:A:208:GLN:O	2.16	0.45
1:A:304:MET:HG2	1:A:309:VAL:HB	1.99	0.45
2:B:272:ILE:CD1	2:B:273:GLU:H	2.29	0.45
2:B:625:LEU:HA	2:B:625:LEU:HD23	1.47	0.45
1:C:149:HIS:O	1:C:151:ALA:N	2.50	0.45
1:C:311:ASP:OD1	1:C:313:ARG:HB3	2.16	0.45
2:B:56:HIS:O	2:B:58:ASN:N	2.50	0.44
1:C:65:GLU:N	1:C:66:GLN:O	2.50	0.44
1:C:124:GLY:HA3	1:C:186:ARG:NH1	2.30	0.44
2:D:113:GLU:O	2:D:114:PRO:C	2.55	0.44
2:D:517:ASP:OD1	2:D:519:LYS:CG	2.64	0.44
1:A:143:LEU:O	1:A:144:ASN:HB3	2.17	0.44
1:A:304:MET:O	1:A:308:GLY:N	2.49	0.44
2:B:221:VAL:O	2:B:221:VAL:HG13	2.17	0.44
2:B:705:ALA:HB2	2:B:763:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:731:GLY:O	2:D:732:VAL:HG12	2.16	0.44
2:B:518:PRO:HG3	2:B:543:ALA:HB2	1.99	0.44
2:D:561:ASN:C	2:D:563:GLN:H	2.20	0.44
2:B:424:GLU:CD	2:B:424:GLU:H	2.21	0.44
1:C:143:LEU:HD22	1:C:250:PHE:CD2	2.53	0.44
2:D:151:LEU:O	2:D:152:LYS:C	2.55	0.44
2:D:183:ASN:C	2:D:185:LEU:H	2.21	0.44
2:D:271:ARG:HD3	2:D:321:HIS:NE2	2.33	0.44
2:D:271:ARG:NH1	2:D:321:HIS:O	2.50	0.44
2:D:532:LEU:O	2:D:534:PRO:HD3	2.16	0.44
2:B:460:ASP:O	2:B:463:GLU:HG2	2.17	0.44
2:B:581:GLN:HE21	2:B:581:GLN:HB3	1.60	0.44
2:B:630:LYS:CB	2:B:631:LEU:HA	2.47	0.44
1:C:105:GLY:CA	2:D:508:GLN:OE1	2.65	0.44
1:C:218:ILE:C	1:C:218:ILE:HD13	2.38	0.44
2:D:621:LEU:HD12	2:D:625:LEU:HD22	1.98	0.44
1:A:204:PRO:HD2	2:B:513:TYR:CE1	2.52	0.44
2:B:499:LYS:HG2	2:B:570:PHE:CE1	2.53	0.44
2:B:540:GLU:HG3	2:B:541:MET:HG3	1.99	0.44
1:C:133:ILE:HD12	2:D:576:PHE:CD1	2.53	0.44
1:A:205:MET:HG2	1:A:206:PHE:N	2.32	0.44
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.85	0.44
2:B:52:GLU:OE2	2:B:52:GLU:HA	2.17	0.44
2:B:56:HIS:O	2:B:57:PRO:C	2.56	0.44
2:D:337:PHE:CZ	2:D:401:PRO:CG	3.00	0.44
2:D:375:ARG:HD3	2:D:375:ARG:HA	1.78	0.44
2:D:416:LEU:HD23	2:D:416:LEU:HA	1.87	0.44
1:A:123:LEU:HD21	2:D:485:MET:HG2	2.00	0.44
1:A:216:THR:HG22	1:A:289:VAL:O	2.18	0.44
2:B:226:VAL:HG11	2:B:328:THR:O	2.17	0.44
2:D:108:ALA:O	2:D:115:SER:HA	2.18	0.44
1:A:199:ASP:OD1	1:A:202:HIS:CD2	2.71	0.44
1:A:299:MET:HA	1:A:299:MET:CE	2.48	0.44
1:C:300:GLU:HB2	1:C:315:PHE:CE1	2.53	0.44
2:B:731:GLY:O	2:B:733:ASN:N	2.51	0.43
2:D:535:SER:N	2:D:536:PRO:HD3	2.33	0.43
2:D:617:LEU:HD12	2:D:617:LEU:HA	1.87	0.43
2:D:625:LEU:CD1	2:D:659:ILE:HD11	2.48	0.43
1:A:150:PRO:O	1:A:154:ASP:HB2	2.18	0.43
2:B:205:ILE:HG13	2:B:394:ILE:HD11	1.99	0.43
2:B:570:PHE:CD1	2:B:570:PHE:C	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:625:LEU:HD13	2:B:634:VAL:CG1	2.48	0.43
2:B:696:GLN:O	2:B:697:ALA:C	2.56	0.43
2:B:774:ILE:C	2:B:776:ALA:N	2.71	0.43
2:D:26:THR:CG2	2:D:32:VAL:HG22	2.48	0.43
1:A:167:ARG:HH11	1:A:167:ARG:HD2	1.65	0.43
1:A:218:ILE:HG12	1:A:292:GLY:HA2	2.00	0.43
1:C:192:ARG:NH2	2:D:571:GLU:OE2	2.52	0.43
2:D:5:GLU:OE1	2:D:18:SER:OG	2.36	0.43
2:D:36:GLU:O	2:D:156:ASN:HA	2.17	0.43
2:D:257:LEU:HD23	2:D:263:PRO:HA	2.00	0.43
2:D:289:LEU:C	2:D:291:ASP:H	2.22	0.43
2:D:427:THR:HG21	2:D:439:GLU:OE2	2.18	0.43
2:D:729:LYS:H	2:D:731:GLY:H	1.65	0.43
1:A:140:PHE:O	1:A:145:ILE:CB	2.67	0.43
1:A:269:VAL:HG12	1:A:270:LEU:N	2.33	0.43
2:B:515:PHE:CD1	2:B:544:MET:HE1	2.42	0.43
2:D:55:GLN:H	2:D:55:GLN:HG2	1.50	0.43
2:D:262:GLN:HA	2:D:263:PRO:HD3	1.76	0.43
2:D:724:LEU:HD21	2:D:740:LEU:HB2	2.00	0.43
1:A:195:ARG:HD2	1:A:206:PHE:CE1	2.53	0.43
2:B:234:MET:O	2:B:234:MET:HG2	2.19	0.43
2:B:284:GLY:HA2	2:B:296:LYS:HE3	2.00	0.43
2:B:545:ARG:HG3	2:B:547:SER:O	2.18	0.43
2:B:661:PHE:O	2:B:682:PHE:HA	2.18	0.43
1:C:29:VAL:HG11	1:C:75:LYS:HB3	1.99	0.43
1:C:194:TYR:CE1	1:C:205:MET:HG3	2.54	0.43
1:C:301:ARG:NE	4:C:999:AMP:N1	2.67	0.43
2:D:241:CYS:HB3	2:D:258:LEU:HD22	1.99	0.43
1:A:156:ASP:HB2	1:A:196:ASN:HB3	1.99	0.43
1:A:263:ASN:CB	1:A:264:GLY:CA	2.92	0.43
2:B:289:LEU:N	2:B:293:THR:O	2.34	0.43
2:B:344:THR:O	2:B:345:GLY:C	2.57	0.43
2:B:622:GLU:HB2	1:C:100:ARG:HD3	1.99	0.43
2:B:629:GLY:CA	2:B:692:ARG:HB2	2.47	0.43
2:B:790:GLN:HG3	2:B:791:ALA:N	2.34	0.43
2:D:1:MET:HB2	2:D:2:LYS:H	1.58	0.43
2:D:147:ILE:HD12	2:D:148:ARG:N	2.34	0.43
2:D:326:ASP:N	2:D:326:ASP:OD1	2.51	0.43
2:B:170:LEU:HD12	2:B:170:LEU:HA	1.86	0.43
2:B:352:LEU:HD12	2:B:352:LEU:HA	1.87	0.43
2:B:522:GLN:CD	2:B:529:GLU:HG3	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:536:PRO:HB2	2:D:537:ILE:HD12	2.01	0.43
1:A:123:LEU:HB3	2:D:483:LEU:HD13	1.99	0.43
2:B:1:MET:O	2:B:1:MET:HG3	2.16	0.43
2:B:55:GLN:HE22	2:B:63:ARG:HH21	1.67	0.43
2:B:225:ASN:ND2	2:B:227:LYS:HG2	2.34	0.43
2:B:629:GLY:O	2:B:630:LYS:O	2.36	0.43
2:B:741:PHE:HB2	2:D:603:GLU:HG3	2.00	0.43
1:C:101:ILE:O	1:C:102:GLU:C	2.57	0.43
2:D:431:ARG:CZ	2:D:437:VAL:HG23	2.48	0.43
2:D:565:ASN:O	2:D:565:ASN:CG	2.57	0.43
2:D:673:LEU:O	2:D:674:ASP:C	2.56	0.43
2:D:678:ARG:O	2:D:678:ARG:HG3	2.18	0.43
2:B:596:ILE:CD1	2:B:612:VAL:HG21	2.36	0.43
2:B:674:ASP:O	2:B:675:LEU:HB2	2.17	0.43
2:D:254:ASN:HD22	2:D:254:ASN:HA	1.66	0.43
1:A:167:ARG:CD	1:A:193:VAL:HG12	2.49	0.43
2:B:142:PRO:O	2:B:144:GLY:N	2.52	0.43
2:B:614:PHE:HA	2:B:680:LEU:HD21	2.00	0.43
2:D:703:PHE:HE2	2:D:766:SER:O	1.98	0.43
2:D:358:HIS:CD2	2:D:362:ARG:NH2	2.87	0.42
2:D:545:ARG:HB2	2:D:547:SER:O	2.19	0.42
2:D:590:LEU:HD12	2:D:686:TRP:CD1	2.54	0.42
2:D:595:VAL:HA	2:D:680:LEU:O	2.19	0.42
2:D:641:ASN:HB3	2:D:644:LEU:HD11	2.00	0.42
2:B:224:ILE:N	2:B:329:GLN:O	2.45	0.42
2:B:715:ALA:O	2:B:717:ASN:N	2.49	0.42
2:B:790:GLN:CG	2:B:791:ALA:N	2.82	0.42
2:D:631:LEU:O	2:D:632:ASN:OD1	2.36	0.42
1:A:201:THR:O	1:A:312:LEU:HD23	2.20	0.42
1:A:218:ILE:HD12	1:A:218:ILE:C	2.39	0.42
2:B:113:GLU:HB2	2:B:114:PRO:HD3	2.00	0.42
2:B:291:ASP:OD1	2:B:293:THR:HG22	2.19	0.42
2:B:309:LYS:HZ1	2:B:321:HIS:CE1	2.37	0.42
1:C:301:ARG:O	1:C:305:LEU:HD23	2.19	0.42
1:C:324:LYS:NZ	1:C:325:GLN:HB3	2.33	0.42
2:D:342:SER:HA	2:D:346:ARG:NH2	2.34	0.42
2:D:624:VAL:O	2:D:626:ASP:N	2.52	0.42
2:B:111:ARG:CG	2:B:111:ARG:NH1	2.82	0.42
2:B:172:ILE:O	2:B:173:ILE:C	2.57	0.42
2:B:774:ILE:O	2:B:778:VAL:HG12	2.19	0.42
4:C:999:AMP:H2'	4:C:999:AMP:N3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:ARG:HB2	2:D:395:THR:HG23	2.01	0.42
2:D:215:ARG:HD3	2:D:369:GLN:HB2	2.01	0.42
2:D:553:LEU:HA	2:D:556:VAL:HG13	2.00	0.42
2:B:138:PRO:O	2:B:139:ALA:C	2.58	0.42
2:B:338:PHE:HB2	2:B:343:ILE:HD11	2.00	0.42
1:C:71:LEU:C	1:C:73:ALA:N	2.72	0.42
1:C:75:LYS:O	1:C:75:LYS:CG	2.51	0.42
1:C:244:ARG:HA	1:C:245:PRO:HD3	1.89	0.42
2:D:17:ASP:HB2	2:D:20:ALA:CB	2.50	0.42
2:D:411:SER:O	2:D:412:LYS:C	2.56	0.42
2:D:741:PHE:HE1	2:D:759:SER:HB3	1.84	0.42
1:A:264:GLY:HA3	1:A:265:LYS:HA	1.77	0.42
2:B:262:GLN:OE1	2:B:369:GLN:NE2	2.50	0.42
2:B:425:GLN:NE2	2:B:469:TYR:HD1	2.17	0.42
2:B:566:ARG:HG2	2:B:566:ARG:O	2.18	0.42
2:B:567:VAL:HG23	2:B:569:ILE:HG23	2.00	0.42
2:D:134:ILE:HG23	2:D:134:ILE:O	2.20	0.42
2:D:583:PRO:O	2:D:584:LEU:HB2	2.20	0.42
2:B:42:PHE:CE1	2:B:147:ILE:HD11	2.55	0.42
2:D:273:GLU:HG2	2:D:306:ASP:OD1	2.19	0.42
1:A:188:ILE:HB	1:A:189:ALA:H	1.76	0.42
2:B:12:VAL:HG12	2:B:185:LEU:HD12	2.02	0.42
1:C:154:ASP:C	1:C:156:ASP:H	2.23	0.42
1:C:219:SER:O	1:C:222:ASN:HB2	2.19	0.42
2:D:246:ILE:HG22	2:D:247:ASP:HB2	2.01	0.42
2:D:537:ILE:HD12	2:D:537:ILE:H	1.82	0.42
2:D:165:ASN:HD22	2:D:165:ASN:N	2.18	0.42
2:D:667:PRO:O	2:D:670:GLU:N	2.52	0.42
1:A:111:ARG:NH1	2:D:490:GLU:OE2	2.53	0.42
3:A:980:PHE:N	4:A:992:AMP:O3'	2.48	0.42
2:B:714:VAL:HG22	2:B:715:ALA:H	1.85	0.42
2:B:734:GLN:H	2:B:734:GLN:HE21	1.68	0.42
2:B:747:LYS:O	2:B:747:LYS:HG2	2.20	0.42
1:C:301:ARG:NH1	4:C:999:AMP:O3P	2.51	0.42
2:D:79:CYS:SG	2:D:80:GLY:N	2.93	0.42
2:D:208:GLU:HB3	2:D:279:ARG:HB3	2.02	0.42
2:D:592:LEU:O	2:D:683:GLU:HA	2.20	0.42
1:A:107:HIS:CD2	1:A:109:VAL:HG13	2.55	0.41
1:A:158:PHE:CZ	1:A:195:ARG:O	2.66	0.41
2:B:311:LEU:HB2	2:B:322:SER:OG	2.20	0.41
1:C:76:ALA:O	1:C:80:SER:OG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:PRO:O	2:D:230:THR:C	2.58	0.41
2:D:461:LEU:HD23	2:D:461:LEU:HA	1.91	0.41
2:D:600:ARG:NH1	2:D:616:ASP:OD2	2.44	0.41
1:A:143:LEU:CD1	1:A:171:SER:HB3	2.49	0.41
1:A:176:ARG:HG3	1:A:176:ARG:HH21	1.85	0.41
1:A:321:ARG:HH21	2:B:562:ARG:HD3	1.85	0.41
2:B:90:VAL:HG11	2:B:119:LEU:HG	2.02	0.41
2:B:207:VAL:HG23	2:B:278:VAL:HB	2.02	0.41
2:B:787:GLU:O	2:B:787:GLU:CG	2.66	0.41
1:C:52:GLU:HA	1:C:53:ARG:HA	1.86	0.41
2:D:116:GLU:HB2	2:D:117:GLY:CA	2.50	0.41
2:D:534:PRO:O	2:D:535:SER:CB	2.64	0.41
1:A:133:ILE:HD12	2:B:576:PHE:HD1	1.80	0.41
2:B:32:VAL:HG23	2:B:32:VAL:O	2.20	0.41
2:B:209:ALA:H	2:B:210:PRO:CD	2.32	0.41
2:B:231:PRO:O	2:B:232:LEU:C	2.59	0.41
2:B:520:VAL:O	2:B:521:GLN:C	2.58	0.41
2:B:528:VAL:O	2:B:529:GLU:HG2	2.20	0.41
2:B:788:ARG:HA	2:B:788:ARG:HH11	1.84	0.41
1:C:59:VAL:CG2	1:C:62:GLU:HG2	2.40	0.41
2:D:53:CYS:O	2:D:54:ALA:C	2.58	0.41
2:D:67:VAL:HB	2:D:77:ILE:HD12	2.03	0.41
2:D:77:ILE:HB	2:D:117:GLY:H	1.85	0.41
2:D:121:SER:H	2:D:124:GLU:HG3	1.85	0.41
2:D:346:ARG:H	2:D:346:ARG:CD	2.32	0.41
2:D:536:PRO:HG3	2:D:542:SER:HB3	2.03	0.41
2:D:790:GLN:NE2	2:D:791:ALA:O	2.53	0.41
1:A:322:PHE:O	1:A:325:GLN:HG2	2.21	0.41
2:B:4:SER:HB3	2:B:7:TRP:CB	2.50	0.41
2:B:790:GLN:HG3	2:B:791:ALA:H	1.85	0.41
2:D:53:CYS:C	2:D:54:ALA:O	2.57	0.41
2:D:345:GLY:H	2:D:346:ARG:NH1	2.12	0.41
2:D:455:MET:HE2	2:D:455:MET:HB2	1.89	0.41
2:D:597:CYS:HB2	2:D:679:THR:HG22	2.03	0.41
2:D:645:HIS:O	2:D:649:SER:HB3	2.20	0.41
1:A:164:ARG:HH11	2:B:584:LEU:HB3	1.86	0.41
2:D:166:ARG:CZ	2:D:166:ARG:HB2	2.50	0.41
2:D:512:THR:HB	2:D:571:GLU:CD	2.41	0.41
2:D:536:PRO:C	2:D:538:SER:H	2.23	0.41
1:A:145:ILE:HB	1:A:146:PRO:O	2.21	0.41
1:A:160:PHE:HE1	1:A:166:LEU:HG	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:THR:HA	2:B:164:PRO:HD3	1.91	0.41
1:C:139:ASN:ND2	1:C:168:THR:H	2.17	0.41
2:D:72:ASP:HB3	2:D:73:ARG:H	1.69	0.41
2:D:517:ASP:OD1	2:D:519:LYS:HG3	2.21	0.41
2:D:278:VAL:HG12	2:D:278:VAL:O	2.19	0.41
1:A:202:HIS:HA	4:A:992:AMP:N6	2.36	0.41
2:B:657:GLU:O	2:B:659:ILE:HD13	2.20	0.41
1:A:101:ILE:H	1:A:101:ILE:HG12	1.59	0.41
2:B:67:VAL:HG22	2:B:77:ILE:HD12	2.03	0.41
2:B:288:VAL:O	2:B:320:GLU:N	2.54	0.41
2:B:790:GLN:CD	2:B:791:ALA:H	2.24	0.41
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.90	0.41
1:C:299:MET:CE	1:C:299:MET:CA	2.96	0.41
2:D:97:ALA:O	2:D:104:LYS:NZ	2.43	0.41
2:D:644:LEU:HD22	2:D:663:GLY:HA3	2.03	0.41
2:B:123:SER:C	2:B:125:LEU:N	2.74	0.41
2:B:635:GLU:HB2	2:B:653:TYR:HB2	2.03	0.41
2:D:17:ASP:CB	2:D:20:ALA:H	2.33	0.41
2:D:224:ILE:H	2:D:224:ILE:HG13	1.70	0.41
2:D:506:GLY:O	2:D:568:ARG:HD3	2.21	0.41
2:D:708:ARG:HD3	2:D:708:ARG:HA	1.75	0.41
2:B:306:ASP:OD1	2:B:308:ASN:CB	2.69	0.40
2:D:682:PHE:CD2	2:D:682:PHE:C	2.94	0.40
1:A:99:ARG:NH2	2:B:606:ASN:OD1	2.55	0.40
2:B:89:ARG:HG2	2:B:141:ALA:HB3	2.02	0.40
1:C:21:VAL:HG12	1:C:24:LEU:HD22	2.04	0.40
1:C:262:LYS:CG	1:C:263:ASN:N	2.85	0.40
2:D:673:LEU:C	2:D:674:ASP:O	2.60	0.40
2:D:778:VAL:CG2	2:D:779:ALA:N	2.84	0.40
1:A:133:ILE:CD1	2:B:576:PHE:CE1	3.04	0.40
2:B:35:VAL:HG12	2:B:158:ILE:HB	2.04	0.40
2:B:89:ARG:CD	2:B:141:ALA:HB3	2.50	0.40
2:B:90:VAL:HG13	2:B:91:ALA:H	1.83	0.40
2:B:432:ARG:HG2	2:B:432:ARG:NH1	2.22	0.40
2:B:739:ASN:HD22	2:B:740:LEU:H	1.69	0.40
2:D:181:VAL:HB	2:D:432:ARG:HG3	2.03	0.40
2:D:316:ILE:HG22	2:D:317:PHE:HB2	2.04	0.40
2:D:524:ILE:O	2:D:643:ALA:HB2	2.21	0.40
2:D:643:ALA:HB1	2:D:669:LEU:HD22	2.03	0.40
2:D:739:ASN:O	2:D:758:ILE:O	2.39	0.40
2:B:280:MET:O	2:B:281:ALA:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:ARG:NH1	2:B:452:ARG:CG	2.60	0.40
2:B:662:VAL:HG13	2:B:682:PHE:CB	2.51	0.40
2:B:668:GLU:N	2:B:668:GLU:CD	2.74	0.40
2:D:173:ILE:HG23	2:D:174:GLY:N	2.37	0.40
2:D:767:ARG:HD3	2:D:769:LEU:HD23	2.02	0.40
1:A:221:THR:HG23	2:B:417:ILE:O	2.22	0.40
1:A:295:PHE:CD2	1:A:295:PHE:C	2.94	0.40
2:B:121:SER:H	2:B:124:GLU:CG	2.35	0.40
2:B:514:SER:O	2:B:545:ARG:HD2	2.22	0.40
1:C:60:ILE:O	1:C:61:ASN:O	2.39	0.40
1:C:167:ARG:HH21	1:C:191:GLY:HA3	1.86	0.40
1:C:169:GLN:OE1	3:C:990:PHE:N	2.55	0.40
1:C:216:THR:O	1:C:217:ASN:C	2.58	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	240/327 (73%)	197 (82%)	31 (13%)	12 (5%)	2 12
1	C	321/327 (98%)	231 (72%)	57 (18%)	33 (10%)	0 2
2	B	793/795 (100%)	631 (80%)	120 (15%)	42 (5%)	2 11
2	D	793/795 (100%)	628 (79%)	106 (13%)	59 (7%)	1 5
All	All	2147/2244 (96%)	1687 (79%)	314 (15%)	146 (7%)	1 6

All (146) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
1	A	167	ARG

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Mol	Chain	Res	Type
1	A	184	PRO
1	A	189	ALA
1	A	217	ASN
2	B	52	GLU
2	B	111	ARG
2	B	132	SER
2	B	139	ALA
2	B	140	ASP
2	B	143	ILE
2	B	209	ALA
2	B	232	LEU
2	B	280	MET
2	B	346	ARG
2	B	564	GLN
2	B	602	GLU
2	B	630	LYS
2	B	677	GLY
2	B	788	ARG
1	C	27	VAL
1	C	48	LEU
1	C	49	PRO
1	C	50	PRO
1	C	51	GLU
1	C	60	ILE
1	C	61	ASN
1	C	62	GLU
1	C	63	ALA
1	C	66	GLN
1	C	67	VAL
1	C	146	PRO
1	C	151	ALA
1	C	184	PRO
1	C	239	LEU
2	D	55	GLN
2	D	56	HIS
2	D	102	ASP
2	D	116	GLU
2	D	118	MET
2	D	140	ASP
2	D	200	ASP
2	D	290	LEU
2	D	566	ARG

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Mol	Chain	Res	Type
2	D	624	VAL
2	D	626	ASP
2	D	627	LEU
2	D	642	PRO
2	D	673	LEU
2	D	674	ASP
2	D	699	GLU
2	D	759	SER
1	A	186	ARG
2	B	18	SER
2	B	71	GLY
2	B	200	ASP
2	B	273	GLU
2	B	345	GLY
2	B	584	LEU
2	B	716	GLU
1	C	54	PRO
1	C	58	ALA
1	C	72	ASN
1	C	76	ALA
1	C	83	LEU
1	C	152	ARG
1	C	217	ASN
1	C	261	GLY
1	C	262	LYS
2	D	54	ALA
2	D	86	GLN
2	D	143	ILE
2	D	320	GLU
2	D	581	GLN
2	D	655	LYS
2	D	747	LYS
2	D	787	GLU
1	A	262	LYS
2	B	566	ARG
2	B	654	LEU
1	C	150	PRO
1	C	197	ASP
2	D	5	GLU
2	D	17	ASP
2	D	58	ASN
2	D	114	PRO

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Mol	Chain	Res	Type
2	D	129	ASP
2	D	134	ILE
2	D	196	GLY
2	D	603	GLU
2	D	625	LEU
2	D	630	LYS
2	D	729	LYS
2	D	732	VAL
1	A	206	PHE
1	A	252	GLU
1	A	263	ASN
2	B	124	GLU
2	B	226	VAL
2	B	285	GLU
2	B	308	ASN
2	B	344	THR
2	B	675	LEU
2	B	697	ALA
2	B	732	VAL
1	C	15	ILE
1	C	65	GLU
1	C	258	ASP
2	D	69	VAL
2	D	165	ASN
2	D	203	LEU
2	D	211	GLU
2	D	321	HIS
2	D	536	PRO
2	D	563	GLN
2	D	632	ASN
2	D	654	LEU
2	D	667	PRO
1	A	188	ILE
2	B	129	ASP
2	B	184	GLN
2	B	270	ASP
2	B	281	ALA
2	B	642	PRO
2	B	779	ALA
1	C	82	ALA
1	C	218	ILE
2	D	144	GLY

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Mol	Chain	Res	Type
2	D	248	ALA
2	D	257	LEU
2	D	441	LYS
2	D	701	SER
2	D	754	LYS
2	B	199	ILE
1	C	59	VAL
1	C	145	ILE
2	D	95	ILE
2	D	535	SER
2	D	537	ILE
1	A	145	ILE
2	B	138	PRO
2	D	229	PRO
2	D	677	GLY
2	B	246	ILE
2	D	429	ILE
2	B	746	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	212/276 (77%)	164 (77%)	48 (23%)	1 4
1	C	240/276 (87%)	202 (84%)	38 (16%)	2 12
2	B	656/663 (99%)	496 (76%)	160 (24%)	0 3
2	D	657/663 (99%)	504 (77%)	153 (23%)	1 3
All	All	1765/1878 (94%)	1366 (77%)	399 (23%)	1 4

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	96	LEU
1	A	99	ARG

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Mol	Chain	Res	Type
1	A	101	ILE
1	A	103	ASN
1	A	106	LEU
1	A	109	VAL
1	A	123	LEU
1	A	127	VAL
1	A	134	GLU
1	A	141	ASP
1	A	145	ILE
1	A	154	ASP
1	A	164	ARG
1	A	165	LEU
1	A	167	ARG
1	A	168	THR
1	A	169	GLN
1	A	171	SER
1	A	173	VAL
1	A	178	MET
1	A	181	GLN
1	A	185	ILE
1	A	186	ARG
1	A	188	ILE
1	A	195	ARG
1	A	199	ASP
1	A	212	LEU
1	A	218	ILE
1	A	223	LEU
1	A	239	LEU
1	A	241	ILE
1	A	244	ARG
1	A	257	VAL
1	A	263	ASN
1	A	268	GLU
1	A	269	VAL
1	A	282	ASN
1	A	283	VAL
1	A	288	GLU
1	A	293	PHE
1	A	302	LEU
1	A	305	LEU
1	A	310	THR
1	A	313	ARG

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Mol	Chain	Res	Type
1	A	317	GLU
1	A	320	LEU
1	A	323	LEU
2	B	1	MET
2	B	6	LEU
2	B	12	VAL
2	B	16	ILE
2	B	23	ASN
2	B	26	THR
2	B	31	GLU
2	B	33	ASP
2	B	38	VAL
2	B	52	GLU
2	B	53	CYS
2	B	56	HIS
2	B	62	LEU
2	B	76	ASP
2	B	77	ILE
2	B	78	VAL
2	B	84	CYS
2	B	85	ARG
2	B	86	GLN
2	B	89	ARG
2	B	103	PHE
2	B	104	LYS
2	B	106	LYS
2	B	111	ARG
2	B	113	GLU
2	B	124	GLU
2	B	127	ILE
2	B	130	ASP
2	B	131	HIS
2	B	134	ILE
2	B	140	ASP
2	B	145	THR
2	B	147	ILE
2	B	152	LYS
2	B	155	ASP
2	B	157	THR
2	B	158	ILE
2	B	159	GLU
2	B	165	ASN

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Mol	Chain	Res	Type
2	B	170	LEU
2	B	175	VAL
2	B	177	ARG
2	B	178	ASP
2	B	184	GLN
2	B	189	GLN
2	B	193	VAL
2	B	207	VAL
2	B	208	GLU
2	B	225	ASN
2	B	227	LYS
2	B	244	ARG
2	B	246	ILE
2	B	249	VAL
2	B	269	LYS
2	B	272	ILE
2	B	285	GLU
2	B	293	THR
2	B	294	GLU
2	B	303	VAL
2	B	311	LEU
2	B	317	PHE
2	B	327	GLU
2	B	342	SER
2	B	344	THR
2	B	352	LEU
2	B	359	ARG
2	B	362	ARG
2	B	370	HIS
2	B	371	LYS
2	B	375	ARG
2	B	378	ARG
2	B	379	LEU
2	B	387	GLU
2	B	391	VAL
2	B	392	ILE
2	B	394	ILE
2	B	396	ASN
2	B	402	LYS
2	B	403	ARG
2	B	407	THR
2	B	408	LEU

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Mol	Chain	Res	Type
2	B	414	ASP
2	B	416	LEU
2	B	424	GLU
2	B	430	LEU
2	B	431	ARG
2	B	432	ARG
2	B	433	LEU
2	B	437	VAL
2	B	438	THR
2	B	445	GLN
2	B	452	ARG
2	B	457	ILE
2	B	472	ASN
2	B	473	ASN
2	B	476	ASP
2	B	477	GLU
2	B	479	VAL
2	B	487	THR
2	B	502	LEU
2	B	512	THR
2	B	515	PHE
2	B	519	LYS
2	B	520	VAL
2	B	533	LEU
2	B	537	ILE
2	B	538	SER
2	B	539	VAL
2	B	540	GLU
2	B	545	ARG
2	B	546	LEU
2	B	548	LEU
2	B	552	LEU
2	B	556	VAL
2	B	563	GLN
2	B	567	VAL
2	B	574	LEU
2	B	575	ARG
2	B	577	VAL
2	B	584	LEU
2	B	586	ILE
2	B	590	LEU
2	B	595	VAL

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Mol	Chain	Res	Type
2	B	611	THR
2	B	612	VAL
2	B	613	ASP
2	B	617	LEU
2	B	618	LYS
2	B	628	THR
2	B	630	LYS
2	B	631	LEU
2	B	641	ASN
2	B	662	VAL
2	B	668	GLU
2	B	671	ARG
2	B	676	ASN
2	B	678	ARG
2	B	685	GLU
2	B	688	LYS
2	B	689	LEU
2	B	700	ILE
2	B	714	VAL
2	B	716	GLU
2	B	724	LEU
2	B	728	LYS
2	B	732	VAL
2	B	733	ASN
2	B	734	GLN
2	B	738	VAL
2	B	739	ASN
2	B	751	GLU
2	B	756	LEU
2	B	760	LEU
2	B	761	ILE
2	B	768	THR
2	B	769	LEU
2	B	770	GLU
2	B	780	LYS
2	B	787	GLU
2	B	788	ARG
1	C	21	VAL
1	C	62	GLU
1	C	65	GLU
1	C	69	GLN
1	C	74	ARG

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Mol	Chain	Res	Type
1	C	75	LYS
1	C	83	LEU
1	C	91	THR
1	C	94	VAL
1	C	96	LEU
1	C	101	ILE
1	C	103	ASN
1	C	111	ARG
1	C	112	THR
1	C	115	ARG
1	C	123	LEU
1	C	126	THR
1	C	155	HIS
1	C	164	ARG
1	C	165	LEU
1	C	181	GLN
1	C	185	ILE
1	C	209	MET
1	C	218	ILE
1	C	238	ASP
1	C	241	ILE
1	C	246	SER
1	C	259	VAL
1	C	262	LYS
1	C	265	LYS
1	C	270	LEU
1	C	291	SER
1	C	302	LEU
1	C	312	LEU
1	C	313	ARG
1	C	320	LEU
1	C	323	LEU
1	C	324	LYS
2	D	1	MET
2	D	18	SER
2	D	19	ASP
2	D	21	LEU
2	D	30	LEU
2	D	36	GLU
2	D	47	VAL
2	D	50	VAL
2	D	52	GLU

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Mol	Chain	Res	Type
2	D	53	CYS
2	D	55	GLN
2	D	62	LEU
2	D	63	ARG
2	D	65	THR
2	D	66	LYS
2	D	67	VAL
2	D	68	ASN
2	D	72	ASP
2	D	74	LEU
2	D	77	ILE
2	D	95	ILE
2	D	102	ASP
2	D	104	LYS
2	D	110	LEU
2	D	111	ARG
2	D	121	SER
2	D	124	GLU
2	D	127	ILE
2	D	129	ASP
2	D	131	HIS
2	D	143	ILE
2	D	152	LYS
2	D	158	ILE
2	D	161	SER
2	D	165	ASN
2	D	172	ILE
2	D	181	VAL
2	D	182	LEU
2	D	198	THR
2	D	199	ILE
2	D	201	ASP
2	D	202	THR
2	D	203	LEU
2	D	211	GLU
2	D	222	LYS
2	D	227	LYS
2	D	244	ARG
2	D	269	LYS
2	D	272	ILE
2	D	276	ILE
2	D	279	ARG

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Mol	Chain	Res	Type
2	D	280	MET
2	D	282	LYS
2	D	290	LEU
2	D	294	GLU
2	D	304	ILE
2	D	308	ASN
2	D	317	PHE
2	D	322	SER
2	D	326	ASP
2	D	327	GLU
2	D	328	THR
2	D	330	ASN
2	D	341	LEU
2	D	348	ARG
2	D	362	ARG
2	D	375	ARG
2	D	379	LEU
2	D	381	ILE
2	D	392	ILE
2	D	394	ILE
2	D	395	THR
2	D	396	ASN
2	D	400	LEU
2	D	402	LYS
2	D	403	ARG
2	D	408	LEU
2	D	423	ASP
2	D	426	VAL
2	D	427	THR
2	D	430	LEU
2	D	437	VAL
2	D	438	THR
2	D	441	LYS
2	D	443	GLU
2	D	445	GLN
2	D	452	ARG
2	D	462	VAL
2	D	473	ASN
2	D	479	VAL
2	D	480	GLN
2	D	487	THR
2	D	510	VAL

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Mol	Chain	Res	Type
2	D	512	THR
2	D	515	PHE
2	D	519	LYS
2	D	522	GLN
2	D	528	VAL
2	D	532	LEU
2	D	537	ILE
2	D	538	SER
2	D	546	LEU
2	D	556	VAL
2	D	560	GLN
2	D	563	GLN
2	D	564	GLN
2	D	566	ARG
2	D	574	LEU
2	D	577	VAL
2	D	583	PRO
2	D	584	LEU
2	D	586	ILE
2	D	590	LEU
2	D	592	LEU
2	D	603	GLU
2	D	609	LYS
2	D	611	THR
2	D	621	LEU
2	D	623	SER
2	D	625	LEU
2	D	628	THR
2	D	630	LYS
2	D	631	LEU
2	D	632	ASN
2	D	639	GLU
2	D	657	GLU
2	D	664	VAL
2	D	668	GLU
2	D	671	ARG
2	D	674	ASP
2	D	678	ARG
2	D	688	LYS
2	D	689	LEU
2	D	691	ASP
2	D	692	ARG

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Mol	Chain	Res	Type
2	D	698	ARG
2	D	699	GLU
2	D	700	ILE
2	D	702	ARG
2	D	708	ARG
2	D	714	VAL
2	D	717	ASN
2	D	732	VAL
2	D	735	VAL
2	D	740	LEU
2	D	760	LEU
2	D	761	ILE
2	D	767	ARG
2	D	768	THR
2	D	771	GLU
2	D	780	LYS
2	D	786	LYS
2	D	790	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	138	HIS
1	A	155	HIS
1	A	169	GLN
1	A	181	GLN
1	A	202	HIS
1	A	207	HIS
1	A	228	HIS
1	A	276	HIS
1	A	282	ASN
1	A	318	ASN
2	B	24	GLN
2	B	86	GLN
2	B	156	ASN
2	B	165	ASN
2	B	183	ASN
2	B	184	GLN
2	B	225	ASN
2	B	254	ASN
2	B	265	HIS

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Mol	Chain	Res	Type
2	B	321	HIS
2	B	350	HIS
2	B	370	HIS
2	B	420	HIS
2	B	521	GLN
2	B	525	HIS
2	B	560	GLN
2	B	581	GLN
2	B	641	ASN
2	B	734	GLN
2	B	739	ASN
2	B	763	GLN
1	C	66	GLN
1	C	69	GLN
1	C	138	HIS
1	C	139	ASN
1	C	149	HIS
1	C	174	GLN
1	C	181	GLN
1	C	207	HIS
1	C	208	GLN
1	C	222	ASN
1	C	240	GLN
1	C	276	HIS
1	C	325	GLN
2	D	56	HIS
2	D	156	ASN
2	D	165	ASN
2	D	225	ASN
2	D	254	ASN
2	D	445	GLN
2	D	473	ASN
2	D	480	GLN
2	D	521	GLN
2	D	525	HIS
2	D	564	GLN
2	D	641	ASN
2	D	763	GLN
2	D	790	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	$\#\|Z\| > 2$
3	PHE	C	990	-	11,12,12	0.72	0	14,15,15	0.96	2 (14%)
3	PHE	A	980	-	11,12,12	0.68	0	14,15,15	0.65	0
4	AMP	A	992	-	22,25,25	1.43	3 (13%)	25,38,38	2.06	6 (24%)
4	AMP	C	999	-	22,25,25	1.42	2 (9%)	25,38,38	1.40	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PHE	C	990	-	-	4/8/8/8	0/1/1/1
3	PHE	A	980	-	-	2/8/8/8	0/1/1/1
4	AMP	A	992	-	-	5/6/26/26	0/3/3/3
4	AMP	C	999	-	-	5/6/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	992	AMP	P-O1P	4.17	1.64	1.50
4	C	999	AMP	P-O1P	4.08	1.63	1.50
4	C	999	AMP	O4'-C1'	3.62	1.46	1.41
4	A	992	AMP	C5-N7	-2.04	1.32	1.39
4	A	992	AMP	P-O3P	2.03	1.62	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	992	AMP	O4'-C1'-C2'	-5.84	98.40	106.93
4	A	992	AMP	N3-C2-N1	-4.82	121.14	128.68
4	C	999	AMP	N3-C2-N1	-4.64	121.42	128.68
4	A	992	AMP	P-O5'-C5'	3.25	127.23	118.30
4	A	992	AMP	O2P-P-O5'	3.16	115.13	106.73
3	C	990	PHE	OXT-C-O	-2.70	117.97	124.09
4	A	992	AMP	O3P-P-O5'	-2.53	100.01	106.73
4	C	999	AMP	C3'-C2'-C1'	2.47	104.69	100.98
3	C	990	PHE	OXT-C-CA	2.18	120.80	113.38
4	A	992	AMP	C2-N1-C6	2.09	122.34	118.75
4	C	999	AMP	P-O5'-C5'	2.06	123.98	118.30

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	990	PHE	N-CA-CB-CG
3	C	990	PHE	C-CA-CB-CG
4	A	992	AMP	C5'-O5'-P-O2P
4	A	992	AMP	C5'-O5'-P-O3P
4	C	999	AMP	C5'-O5'-P-O1P
4	C	999	AMP	C5'-O5'-P-O2P
4	C	999	AMP	C5'-O5'-P-O3P
4	C	999	AMP	O4'-C4'-C5'-O5'
4	C	999	AMP	C3'-C4'-C5'-O5'
4	A	992	AMP	O4'-C4'-C5'-O5'
4	A	992	AMP	C3'-C4'-C5'-O5'
3	A	980	PHE	CA-CB-CG-CD2
3	A	980	PHE	CA-CB-CG-CD1
3	C	990	PHE	OXT-C-CA-CB
3	C	990	PHE	O-C-CA-CB
4	A	992	AMP	C4'-C5'-O5'-P

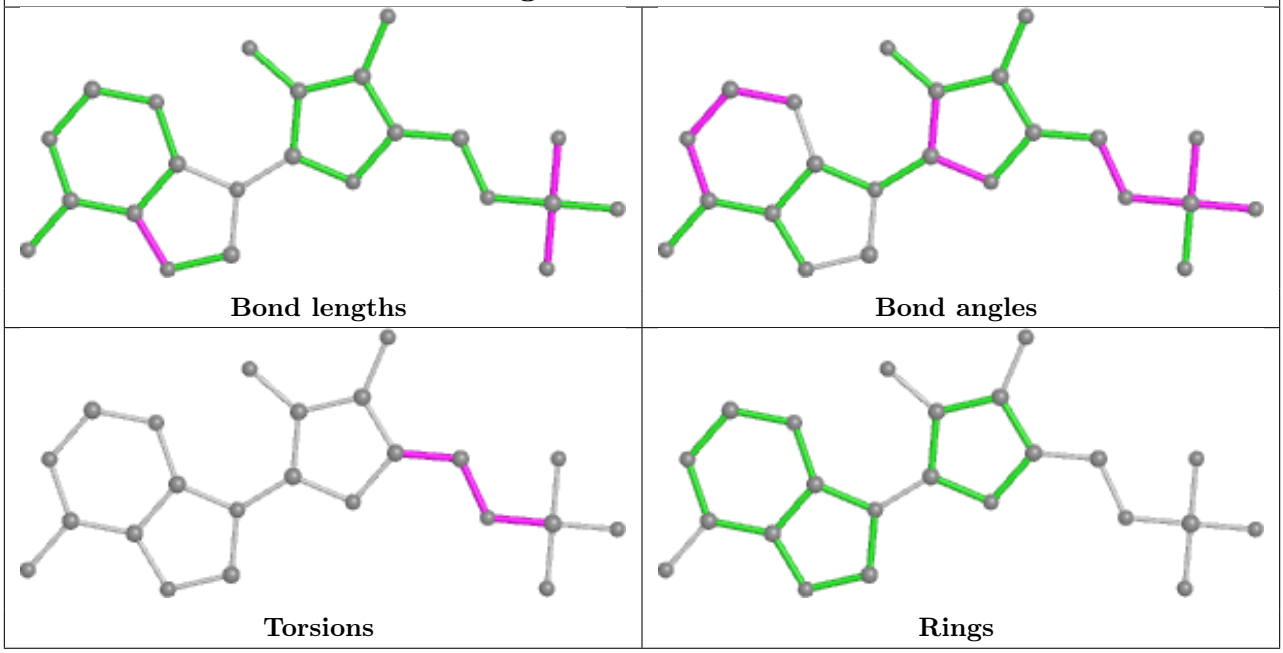
There are no ring outliers.

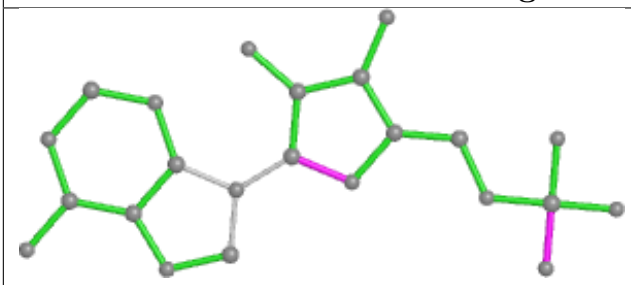
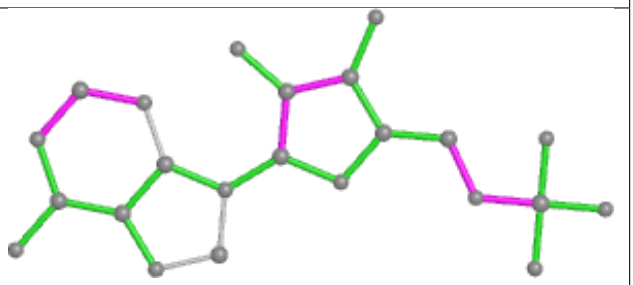
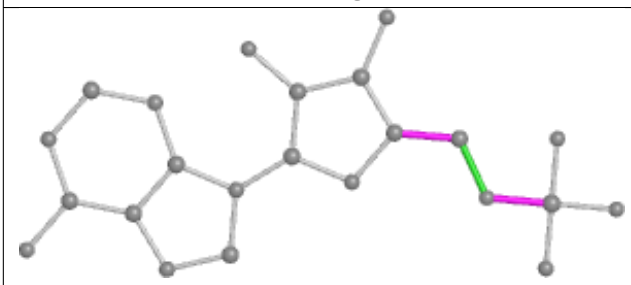
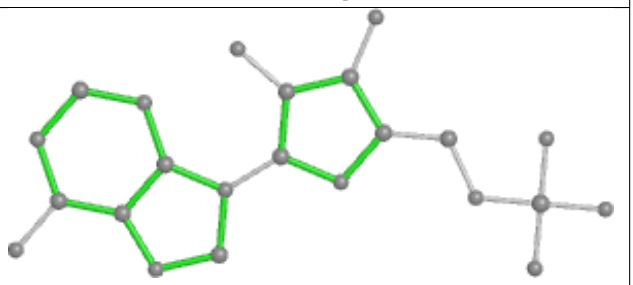
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	990	PHE	1	0
3	A	980	PHE	2	0
4	A	992	AMP	9	0
4	C	999	AMP	9	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 A 992



Ligand AMP C 999	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	242/327 (74%)	-0.19	3 (1%) 79 53	50, 63, 87, 145	0
1	C	323/327 (98%)	0.36	28 (8%) 10 3	36, 89, 164, 169	8 (2%)
2	B	795/795 (100%)	-0.21	3 (0%) 92 78	51, 89, 128, 148	0
2	D	795/795 (100%)	-0.03	9 (1%) 80 55	58, 97, 132, 148	0
All	All	2155/2244 (96%)	-0.06	43 (1%) 65 36	36, 90, 138, 169	8 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	SER	5.8
1	C	5	ALA	4.7
1	C	18	ALA	4.7
1	C	59	VAL	4.4
1	C	29	VAL	4.2
1	C	40	LEU	4.1
1	C	11	ALA	4.0
2	D	201	ASP	4.0
1	C	26	ASN	3.8
1	C	15	ILE	3.7
1	C	55	ALA	3.6
1	C	261	GLY	3.5
1	C	31	TYR	3.4
1	A	264	GLY	3.4
1	C	28	ARG	3.3
1	C	58	ALA	3.3
1	C	56	ALA	3.3
1	C	54	PRO	3.1
2	B	781	CYS	3.1
1	C	43	THR	2.9
1	A	87	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	44	THR	2.7
2	D	211	GLU	2.6
2	D	114	PRO	2.6
1	C	41	GLN	2.5
1	C	57	GLY	2.4
1	C	243	PHE	2.4
1	C	45	LEU	2.4
1	A	88	ALA	2.3
1	C	163	THR	2.3
1	C	254	SER	2.3
2	D	75	LEU	2.2
2	D	202	THR	2.2
1	C	60	ILE	2.2
2	D	71	GLY	2.2
2	D	109	LYS	2.2
1	C	39	THR	2.2
1	C	62	GLU	2.1
2	B	131	HIS	2.1
1	C	16	SER	2.1
2	B	785	LEU	2.1
2	D	91	ALA	2.1
2	D	345	GLY	2.1

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
4	AMP	C	999	23/23	0.80	0.34	137,145,147,147	0

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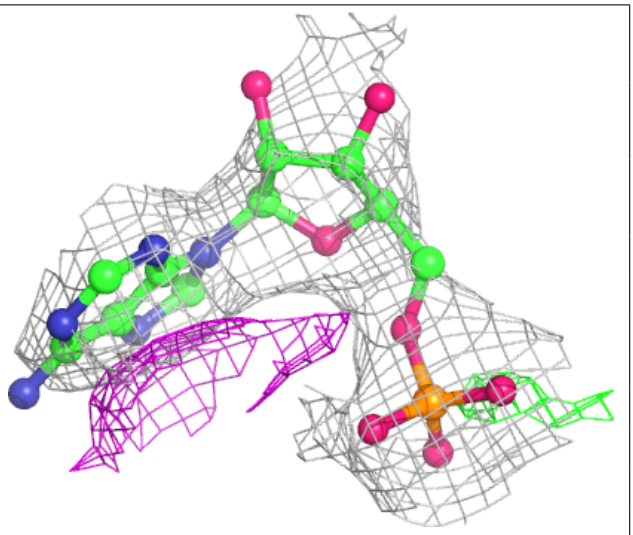
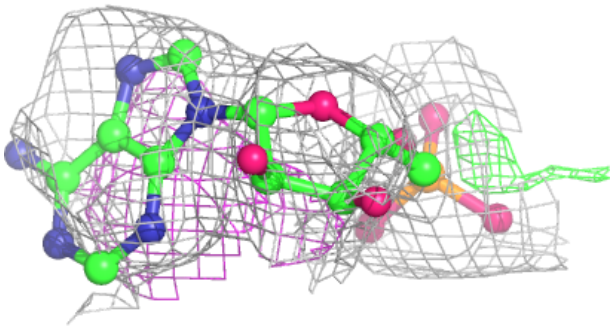
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PHE	A	980	12/12	0.89	0.38	73,80,87,87	0
4	AMP	A	992	23/23	0.91	0.37	96,99,101,101	0
3	PHE	C	990	12/12	0.93	0.30	95,98,99,99	0

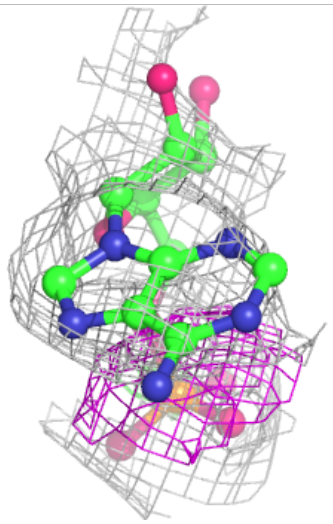
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP C 999:

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

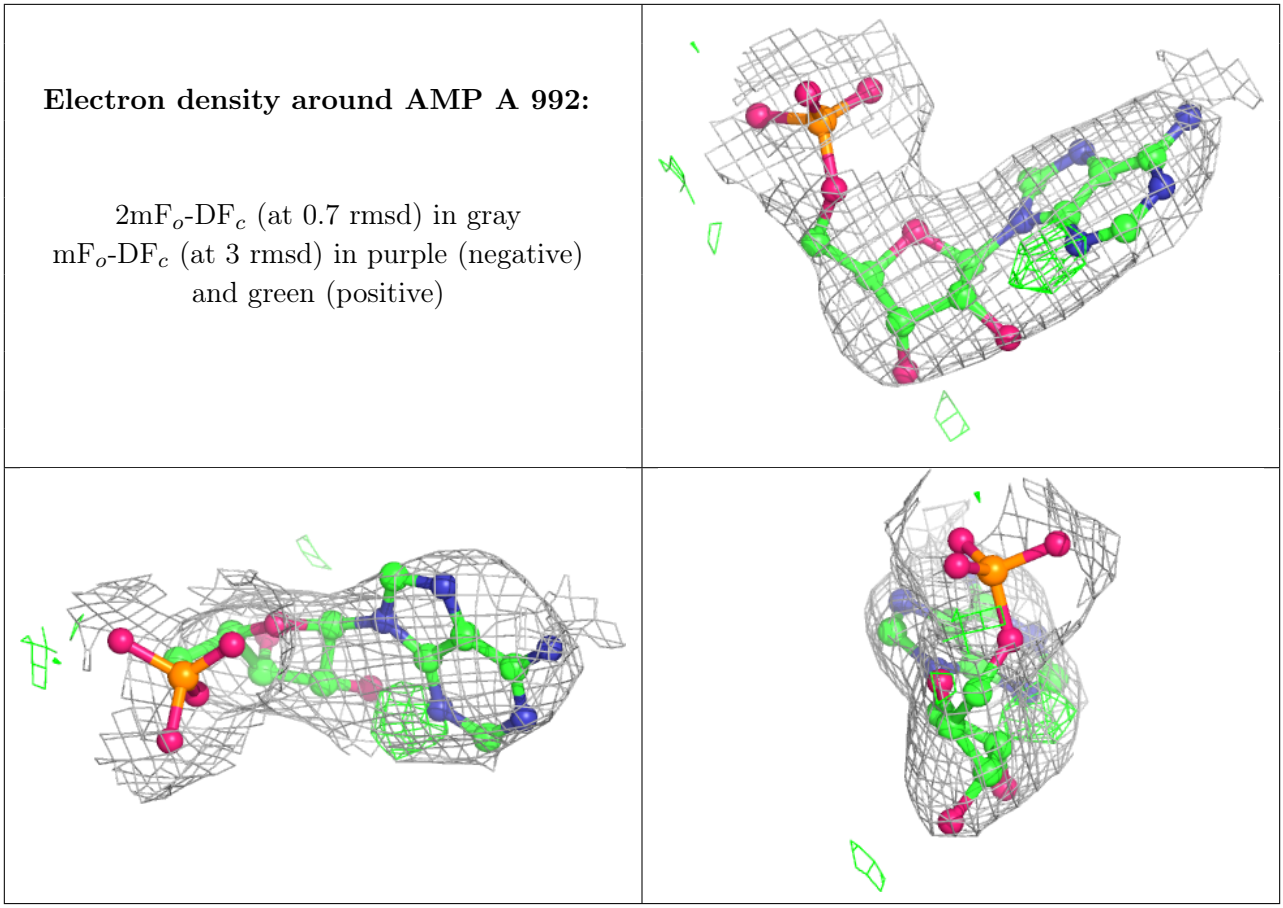






Electron density around AMP A 992:

$2mF_o$-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

There are no such residues in this entry.