



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:06 AM UTC

PDB ID : 3PCO / pdb_00003pco
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

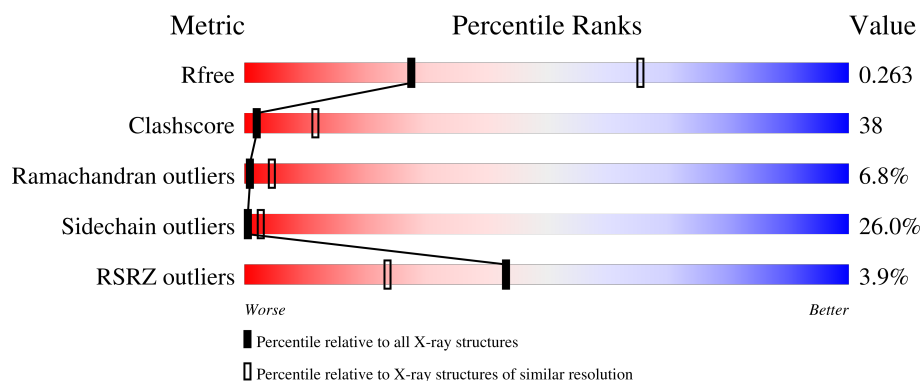
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	2% 28% 30% 14% 26%
1	C	327	8% 38% 43% 13%
2	B	795	% 41% 39% 17%
2	D	795	5% 42% 39% 16%

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.

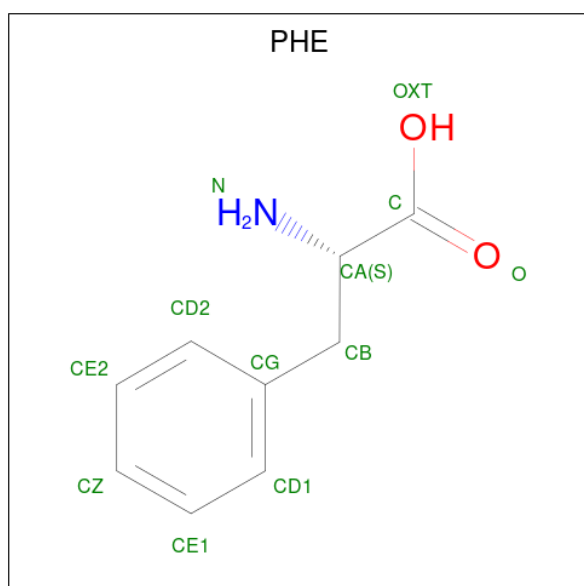
- Molecule 1 is a protein called Phenylalanyl-tRNA synthetase, alpha subunit.

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.

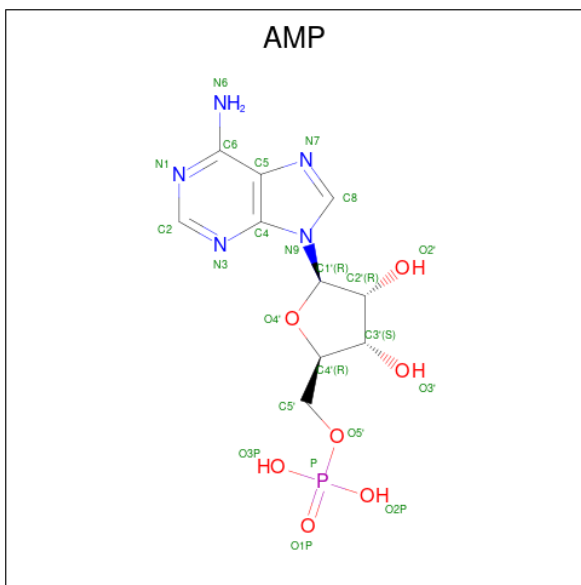
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	795	Total	C	N	O	S	0	0	0
			6111	3845	1081	1158	27			
2	D	795	Total	C	N	O	S	0	0	0
			6117	3848	1081	1161	27			

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

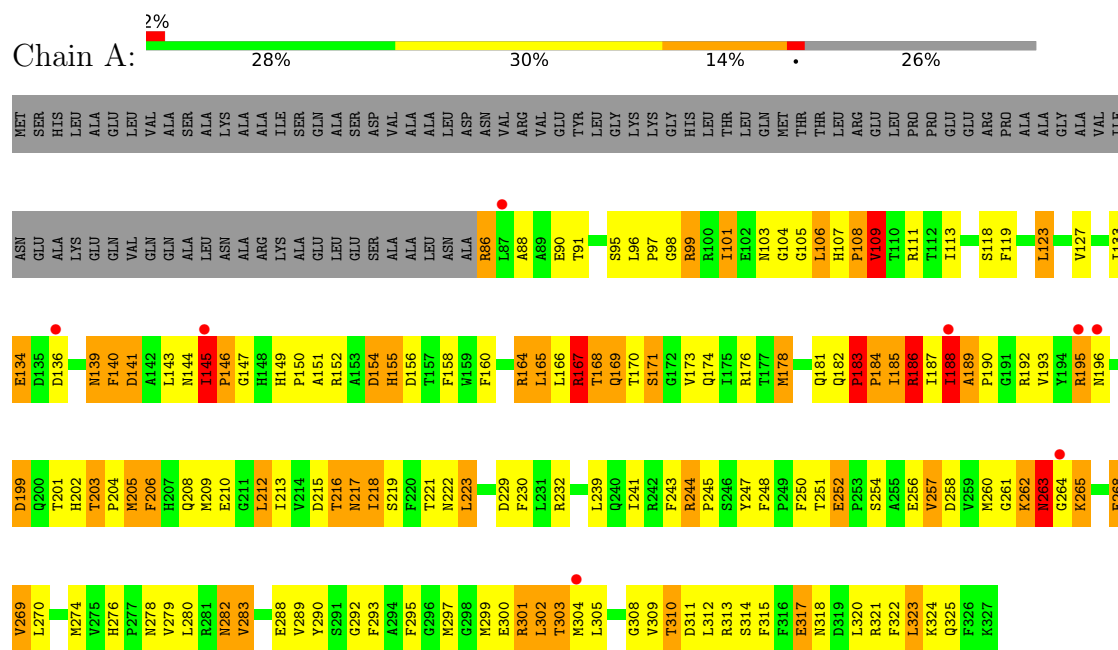


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

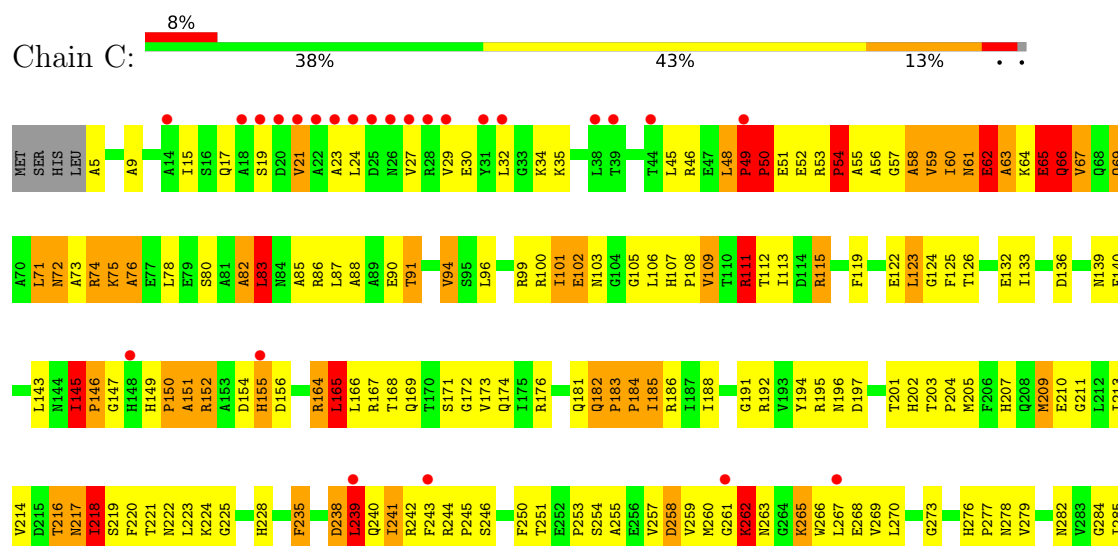
3 Residue-property plots

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

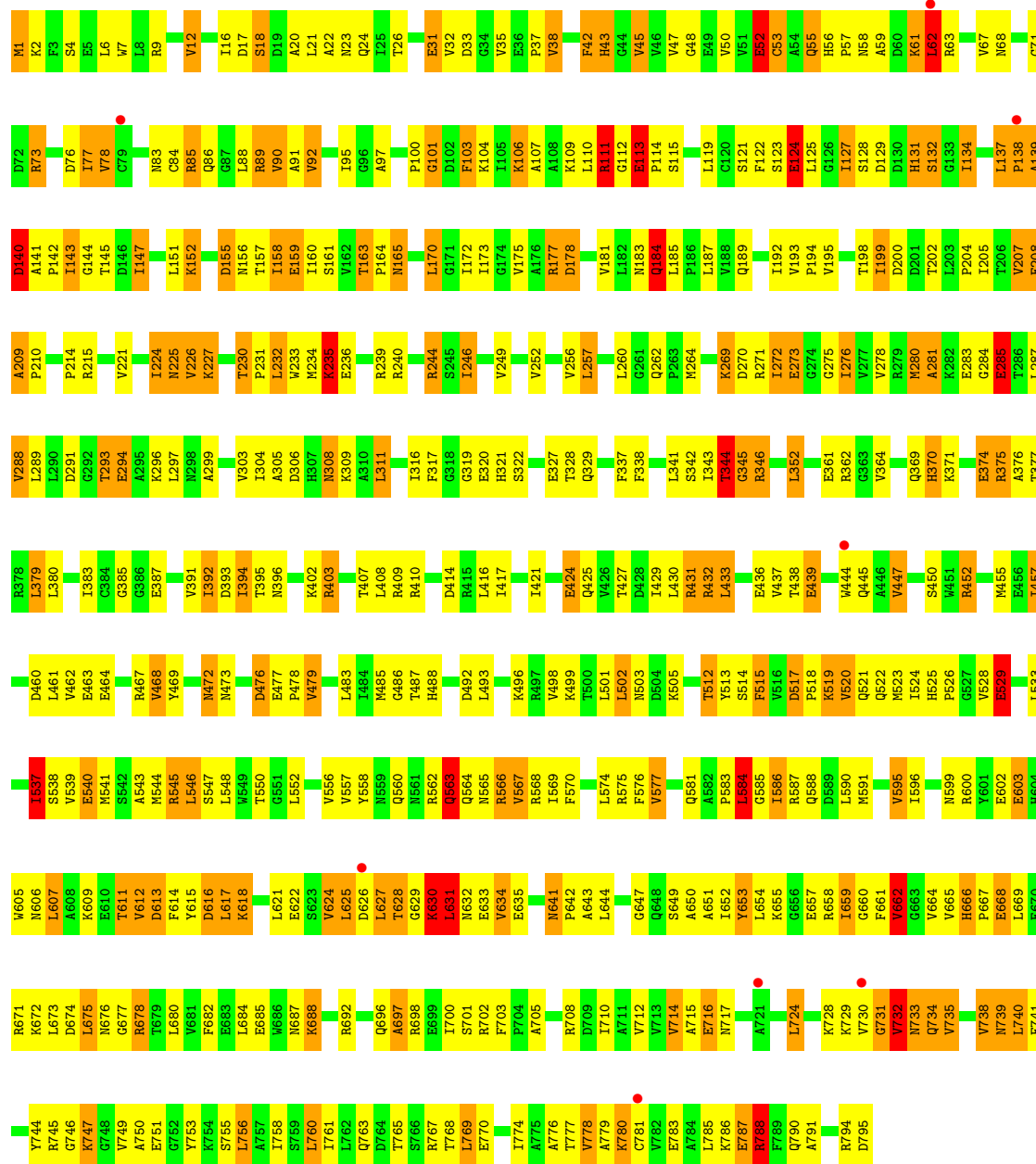


- Molecule 1: Phenylalanyl-tRNA synthetase, alpha subunit

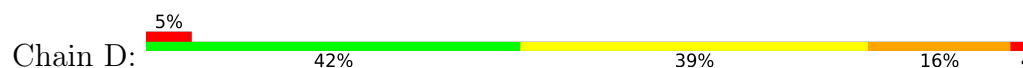


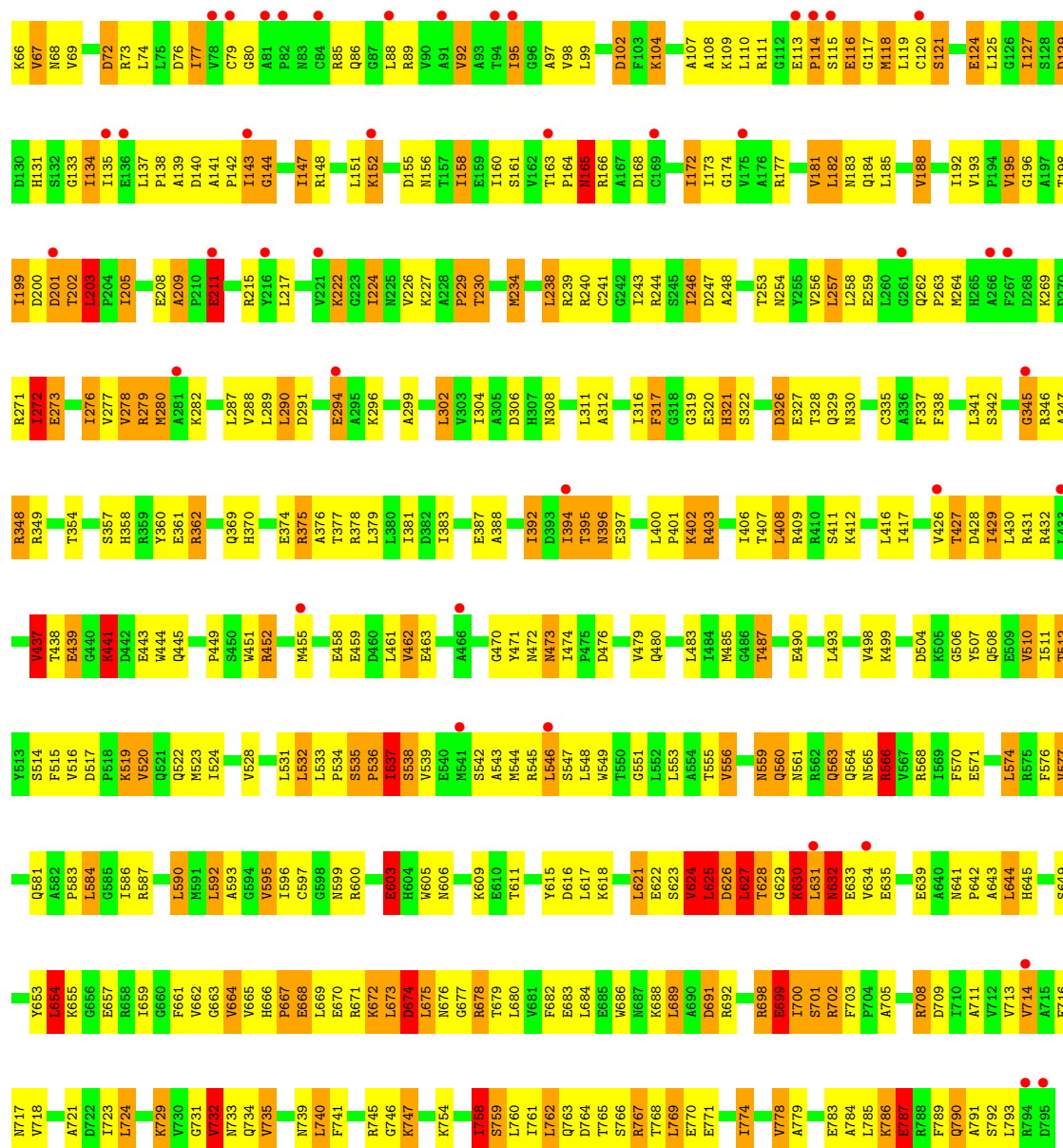


• Molecule 2: Phenylalanyl-tRNA synthetase, beta chain



• Molecule 2: Phenylalanyl-tRNA synthetase, beta chain





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.300 0.267 , 0.263	Depositor DCC
R_{free} test set	2981 reflections (4.98%)	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)	0.28 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.92	1/2016 (0.0%)	1.32	25/2730 (0.9%)
1	C	0.83	0/2516	1.20	17/3412 (0.5%)
2	B	0.87	0/6212	1.23	40/8432 (0.5%)
2	D	0.81	2/6218 (0.0%)	1.16	31/8440 (0.4%)
All	All	0.85	3/16962 (0.0%)	1.21	113/23014 (0.5%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	654	LEU	N-CA	5.91	1.53	1.46
1	A	203	THR	CA-C	5.57	1.58	1.52
2	D	188	VAL	CA-CB	5.01	1.59	1.53

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	627	LEU	N-CA-C	-12.15	98.43	113.01
2	B	624	VAL	N-CA-C	-10.22	100.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	GLU	N-CA-C	8.22	120.24	111.28
2	D	758	ILE	N-CA-C	7.95	121.26	113.71
2	B	476	ASP	N-CA-C	7.83	122.59	112.26
2	B	653	TYR	N-CA-C	7.71	122.73	111.02
1	C	49	PRO	N-CA-CB	7.60	110.46	103.08
1	A	106	LEU	N-CA-C	7.58	119.73	110.41
1	A	105	GLY	N-CA-C	-7.56	100.68	112.85
2	B	669	LEU	N-CA-C	-7.49	103.20	111.36
1	C	302	LEU	N-CA-CB	7.42	120.74	109.91
2	D	36	GLU	CA-C-N	-7.27	112.14	119.92
2	D	36	GLU	C-N-CA	-7.27	112.14	119.92
2	B	20	ALA	N-CA-C	-7.15	103.22	112.23
1	A	244	ARG	CB-CA-C	7.11	119.87	109.48
2	D	675	LEU	N-CA-C	7.11	120.22	109.63
2	B	101	GLY	N-CA-C	-7.01	105.06	114.95
2	B	97	ALA	N-CA-C	7.00	120.14	110.35
1	C	54	PRO	N-CA-CB	6.89	110.48	103.25
1	A	164	ARG	N-CA-C	-6.74	99.04	109.76
1	A	215	ASP	CB-CA-C	-6.71	99.16	110.43
1	C	50	PRO	N-CA-CB	6.70	110.29	103.25
1	A	303	THR	N-CA-C	6.57	118.10	111.07
2	D	202	THR	N-CA-C	6.57	119.41	109.23
1	A	183	PRO	N-CA-C	6.53	118.67	110.70
2	D	523	MET	N-CA-C	-6.51	104.26	111.82
2	B	537	ILE	CB-CA-C	-6.49	101.59	112.16
2	D	769	LEU	N-CA-C	6.47	119.62	110.23
1	C	302	LEU	N-CA-C	-6.46	103.92	110.97
2	B	62	LEU	N-CA-C	6.40	119.88	110.59
1	A	164	ARG	CB-CA-C	6.36	120.20	109.84
2	B	529	GLU	N-CA-C	6.35	119.06	109.41
2	B	624	VAL	CB-CA-C	-6.34	103.72	112.02
1	A	244	ARG	CA-C-N	6.33	126.24	119.85
1	A	244	ARG	C-N-CA	6.33	126.24	119.85
2	B	595	VAL	CB-CA-C	-6.32	101.08	110.82
1	C	102	GLU	N-CA-C	-6.29	102.06	110.24
1	A	245	PRO	CB-CA-C	-6.29	102.75	110.98
2	D	230	THR	CA-C-N	6.25	126.01	119.76
2	D	230	THR	C-N-CA	6.25	126.01	119.76
2	D	789	PHE	CB-CA-C	-6.13	109.51	116.63
2	B	607	LEU	N-CA-C	6.08	118.14	110.24
1	A	205	MET	N-CA-C	-6.02	100.17	109.14
1	C	182	GLN	CA-C-N	-5.98	114.22	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	GLN	C-N-CA	-5.98	114.22	120.38
1	A	139	ASN	N-CA-C	-5.95	104.38	111.69
1	A	141	ASP	N-CA-C	5.92	118.69	111.82
1	A	184	PRO	N-CA-C	-5.92	100.28	112.47
2	B	666	HIS	CA-C-N	5.87	127.18	119.84
2	B	666	HIS	C-N-CA	5.87	127.18	119.84
1	C	235	PHE	N-CA-C	-5.87	101.33	110.42
2	D	516	VAL	N-CA-C	5.87	115.69	108.53
1	A	140	PHE	CB-CA-C	-5.79	98.89	110.42
2	B	563	GLN	N-CA-C	-5.78	94.82	111.00
1	A	223	LEU	N-CA-C	-5.78	104.90	111.14
1	A	140	PHE	N-CA-C	5.74	123.02	110.80
1	C	165	LEU	N-CA-C	5.73	117.79	109.07
1	C	183	PRO	N-CA-C	5.71	117.66	110.70
1	A	109	VAL	N-CA-CB	5.70	118.30	110.54
2	B	603	GLU	N-CA-C	5.70	118.15	111.02
2	D	203	LEU	N-CA-C	5.69	122.39	109.81
2	B	747	LYS	N-CA-C	5.66	119.29	112.38
2	D	417	ILE	N-CA-C	-5.62	106.33	111.67
2	B	485	MET	N-CA-C	5.60	120.24	113.41
2	D	98	VAL	N-CA-C	5.60	116.05	107.77
2	B	616	ASP	N-CA-C	-5.55	104.87	111.03
2	D	118	MET	N-CA-C	5.54	122.61	110.80
2	D	566	ARG	N-CA-C	-5.51	99.05	110.80
2	B	163	THR	CA-C-N	5.47	126.68	119.84
2	B	163	THR	C-N-CA	5.47	126.68	119.84
2	D	205	ILE	N-CA-C	5.47	115.42	106.72
2	B	735	VAL	N-CA-C	5.47	115.73	107.75
2	D	624	VAL	CB-CA-C	-5.46	102.34	111.29
2	B	745	ARG	N-CA-C	5.41	121.44	114.56
2	B	496	LYS	N-CA-C	-5.41	105.55	111.82
2	B	662	VAL	CB-CA-C	-5.40	101.36	110.71
2	D	163	THR	CA-C-N	5.37	126.55	119.84
2	D	163	THR	C-N-CA	5.37	126.55	119.84
2	D	209	ALA	CA-C-N	5.34	124.53	118.97
2	D	209	ALA	C-N-CA	5.34	124.53	118.97
2	B	45	VAL	N-CA-C	-5.33	100.78	108.71
2	B	618	LYS	N-CA-C	-5.30	105.50	111.28
2	B	486	GLY	CA-C-N	-5.29	115.08	123.12
2	B	486	GLY	C-N-CA	-5.29	115.08	123.12
2	D	272	ILE	N-CA-C	5.28	117.97	112.90
2	B	517	ASP	CA-C-N	-5.27	113.60	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	517	ASP	C-N-CA	-5.27	113.60	119.19
2	B	95	ILE	N-CA-C	5.26	115.70	110.23
1	A	216	THR	N-CA-C	-5.26	99.60	110.80
2	B	235	LYS	N-CA-C	-5.26	99.60	110.80
2	B	492	ASP	CB-CA-C	5.20	118.22	109.48
1	A	155	HIS	N-CA-C	-5.19	101.67	109.15
2	D	58	ASN	N-CA-C	-5.18	99.76	110.80
2	D	718	VAL	CA-C-N	-5.17	114.38	119.92
2	D	718	VAL	C-N-CA	-5.17	114.38	119.92
2	B	550	THR	N-CA-C	-5.15	105.74	111.36
2	D	354	THR	CB-CA-C	-5.15	100.81	109.83
1	A	139	ASN	CB-CA-C	5.15	120.12	110.70
2	D	520	VAL	N-CA-C	5.10	115.87	110.72
1	A	310	THR	CB-CA-C	-5.08	102.05	110.68
2	B	731	GLY	N-CA-C	-5.07	108.06	115.72
1	C	216	THR	N-CA-C	-5.05	103.38	110.50
1	C	184	PRO	N-CA-C	-5.05	102.06	112.47
2	B	702	ARG	N-CA-C	-5.05	106.96	113.02
1	C	111	ARG	N-CA-C	-5.04	105.67	111.07
2	D	437	VAL	N-CA-C	5.04	115.16	108.11
1	A	108	PRO	CA-C-N	-5.03	113.57	120.46
1	A	108	PRO	C-N-CA	-5.03	113.57	120.46
2	B	660	GLY	N-CA-C	5.03	117.52	110.38
2	D	487	THR	N-CA-C	5.02	116.95	108.96
2	D	409	ARG	N-CA-C	5.01	116.91	109.25
1	C	66	GLN	CA-C-N	5.00	130.98	121.97
1	C	66	GLN	C-N-CA	5.00	130.98	121.97

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

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Mol	Chain	Res	Type	Group
1	C	182	GLN	Peptide
1	C	183	PRO	Peptide
1	C	262	LYS	Peptide
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	223	0
1	C	2462	0	2307	229	0
2	B	6111	0	6166	436	0
2	D	6117	0	6169	445	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	1265	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 38.

All (1265) 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	1.39
1:C:58:ALA:HB1	1:C:60:ILE:CG2	1.58	1.33
2:D:55:GLN:HB2	2:D:56:HIS:C	1.56	1.29
2:D:631:LEU:HD12	2:D:632:ASN:N	1.47	1.27
1:A:155:HIS:CD2	1:A:168:THR:HG21	1.76	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:104:GLY:O	2:B:503:ASN:CG	1.88	1.17
1:C:239:LEU:HB3	1:C:240:GLN:HA	1.24	1.17
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
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:55:GLN:CB	2:D:56:HIS:C	2.31	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
1:A:140:PHE:C	1:A:145:ILE:HG12	1.84	1.01
2:B:537:ILE:H	2:B:537:ILE:CD1	1.73	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:299:MET:HE2	1:C:299:MET:HA	1.44	0.98
1:C:58:ALA:HB1	1:C:60:ILE:HG22	0.98	0.98
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: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
2:D:375:ARG:HH11	2:D:375:ARG:CG	1.78	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:D:449:PRO:HD2	2:D:455:MET:HE1	1.46	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:600:ARG:NH1	2:B:616:ASP:CG	2.27	0.92
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
1:A:166:LEU:O	1:A:167:ARG:C	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD11	2:B:544:MET:HE3	1.54	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
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: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
1:A:166:LEU:HD11	2:B:544:MET:HE1	1.54	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
1:C:59:VAL:N	1:C:60:ILE:C	2.33	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: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
1:C:59:VAL:H	1:C:60:ILE:C	1.84	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
2:D:626:ASP:C	2:D:628:THR:H	1.80	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
1:C:59:VAL:CA	1:C:60:ILE:C	2.50	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:B:264:MET:HE1	2:B:376:ALA:HB2	1.60	0.83
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
1:C:58:ALA:C	1:C:60:ILE:CB	2.44	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:626:ASP:C	2:D:628:THR:N	2.32	0.83
2:D:205:ILE:HG22	2:D:276:ILE:HB	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLU:HB3	1:A:312:LEU:CD1	2.10	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
1:A:140:PHE:O	1:A:145:ILE:CG1	2.27	0.81
2:B:600:ARG:HH11	2:B:616:ASP:CG	1.89	0.81
1:C:59:VAL:HG13	1:C:59:VAL:O	1.80	0.81
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
2:D:510:VAL:O	2:D:571:GLU:HG3	1.80	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
1:A:136:ASP:CG	1:A:152:ARG:HH22	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:VAL:HB	2:D:158:ILE:HD11	1.66	0.77
2:D:127:ILE:C	2:D:127:ILE:HD13	2.10	0.76
2:B:56:HIS:HB3	2:B:63:ARG:H	1.51	0.76
2:D:515:PHE:HD1	2:D:544:MET:HE1	1.49	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
1:A:299:MET:HE2	1:A:299:MET:HA	1.66	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
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
1:C:209:MET:HG2	1:C:297:MET:HE3	1.68	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:145:ILE:HG22	1:A:146:PRO:C	2.13	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:C:166:LEU:HD11	2:D:544:MET:HE1	1.70	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
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
1:C:146:PRO:O	1:C:152:ARG:NE	2.21	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:O	2:B:503:ASN:HB3	1.89	0.72
2:D:624:VAL:HG12	2:D:625:LEU:N	2.02	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: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
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:B:264:MET:HE1	2:B:376:ALA:CB	2.18	0.71
2:D:57:PRO:HB3	2:D:59:ALA:O	1.90	0.71
1:C:61:ASN:O	1:C:62:GLU:C	2.33	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:B:24:GLN:HE22	2:B:183:ASN:CG	1.98	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:A:166:LEU:C	1:A:167:ARG:O	2.34	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:C:58:ALA:CA	1:C:60:ILE:CG2	2.70	0.69
2:B:139:ALA:C	2:B:141:ALA:H	2.00	0.69
2:D:195:VAL:HG21	2:D:377:THR:HB	1.74	0.69
1:C:59:VAL:HA	1:C:60:ILE:C	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ILE:CG2	2:B:276:ILE:HB	2.24	0.68
2:B:462:VAL:O	2:B:463:GLU:C	2.35	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
2:B:515:PHE:HD1	2:B:544:MET:HE1	1.59	0.68
1:A:158:PHE:CZ	2:B:537:ILE:HG13	2.29	0.67
2:B:427:THR:HG21	2:B:439:GLU:CD	2.18	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:729:LYS:C	2:D:731:GLY:H	2.01	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
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:647:GLY:CA	1:C:91:THR:HB	2.25	0.66
1:C:65:GLU:HA	1:C:66:GLN:C	2.20	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
2:D:626:ASP:O	2:D:627:LEU:C	2.37	0.66
1:A:145:ILE:CG2	1:A:146:PRO:C	2.68	0.66
2:D:115:SER:C	2:D:116:GLU:O	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:631:LEU:C	2:D:633:GLU:H	2.05	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:111:ARG:C	2:D:113:GLU:H	2.03	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:630:LYS:HB3	2:B:631:LEU:C	2.22	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
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
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
1:C:300:GLU:H	1:C:300:GLU:CD	2.05	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:631:LEU:CG	2:B:632:ASN:N	2.51	0.64
1:A:166:LEU:CD1	2:B:544:MET:HE1	2.27	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
1:C:188:ILE:HB	1:C:209:MET:HE2	1.80	0.63
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:C:62:GLU:C	1:C:64:LYS:H	2.05	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:62:GLU:C	1:C:64:LYS:N	2.57	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
1:C:60:ILE:O	1:C:61:ASN:C	2.42	0.63
2:D:306:ASP:OD2	2:D:306:ASP:C	2.42	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
1:C:299:MET:HE2	1:C:299:MET:CA	2.26	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: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
2:D:319:GLY:C	2:D:321:HIS:H	2.05	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
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
1:A:170:THR:C	1:A:210:GLU:HG3	2.24	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
2:D:786:LYS:HD2	2:D:791:ALA:CB	2.27	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
1:C:17:GLN:C	1:C:19:SER:H	2.06	0.61
1:C:277:PRO:HG3	2:D:459:GLU:CD	2.25	0.61
2:D:56:HIS:HE1	2:D:58:ASN:HB3	1.55	0.61
2:D:253:THR:CG2	2:D:264:MET:HB2	2.28	0.61
2:D:449:PRO:CD	2:D:455:MET:HE1	2.25	0.61
1:A:205:MET:O	1:A:206:PHE:HB3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:HG13	1:A:302:LEU:CD1	2.31	0.61
1:A:295:PHE:CE2	1:A:297:MET:HE2	2.36	0.61
1:C:225:GLY:HA2	2:D:476:ASP:HB3	1.83	0.61
2:D:115:SER:O	2:D:116:GLU:C	2.43	0.61
2:B:626:ASP:C	2:B:629:GLY:H	2.09	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: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:139:ALA:C	2:B:141:ALA:N	2.59	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: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:B:455:MET:HE3	2:B:461:LEU:CD2	2.32	0.60
2:D:659:ILE:HD12	2:D:684:LEU:HD22	1.83	0.60
2:B:644:LEU:HD13	2:B:649:SER:CB	2.27	0.60
1:A:252:GLU:OE2	2:B:463:GLU:CD	2.45	0.60
2:B:576:PHE:CD1	2:B:588:GLN:HG2	2.37	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:B:294:GLU:CD	2:B:294:GLU:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:641:ASN:C	2:B:643:ALA:H	2.10	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
1:C:171:SER:HA	1:C:210:GLU:CD	2.28	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:C:299:MET:HA	1:C:299:MET:CE	2.27	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:B:787:GLU:O	2:B:787:GLU:HG3	2.03	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
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
1:A:270:LEU:C	1:A:270:LEU:HD12	2.29	0.58
2:D:127:ILE:C	2:D:127:ILE:CD1	2.76	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
2:B:600:ARG:HH12	2:B:616:ASP:CG	2.12	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:B:457:ILE:HG22	2:B:460:ASP:CG	2.27	0.58
2:D:713:VAL:O	2:D:714:VAL:HG23	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:729:LYS:C	2:D:731:GLY:N	2.63	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
1:C:71:LEU:C	1:C:73:ALA:H	2.13	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:606:ASN:CG	2:D:606:ASN:O	2.46	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
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
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:344:THR:HA	2:B:361:GLU:CD	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:624:VAL:O	2:D:625:LEU:C	2.46	0.56
1:A:201:THR:C	1:A:312:LEU:HD23	2.29	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
1:C:185:ILE:HD13	1:C:185:ILE:C	2.30	0.56
2:D:142:PRO:C	2:D:144:GLY:H	2.13	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
2:D:55:GLN:C	2:D:56:HIS:O	2.48	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:55:GLN:C	2:B:56:HIS:CG	2.84	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:522:GLN:CD	2:B:529:GLU:HG3	2.31	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:613:ASP:OD2	2:B:613:ASP:C	2.49	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
1:C:87:LEU:O	1:C:91:THR:CG2	2.54	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
1:A:118:SER:O	1:A:119:PHE:C	2.49	0.55
1:A:86:ARG:HG2	1:A:90:GLU:CD	2.31	0.55
2:B:202:THR:CG2	2:B:392:ILE:HD11	2.36	0.55
1:C:132:GLU:CD	2:D:574:LEU:HD11	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:672:LYS:O	2:D:674:ASP:CG	2.49	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: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:B:687:ASN:OD1	2:B:687:ASN:C	2.49	0.54
2:D:617:LEU:HD23	2:D:662:VAL:HG23	1.89	0.54
2:B:123:SER:C	2:B:125:LEU:H	2.15	0.54
1:C:149:HIS:O	1:C:150:PRO:C	2.50	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:NH2	2:B:512:THR:O	2.41	0.54
1:A:230:PHE:HB2	2:D:485:MET:HE1	1.88	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:583:PRO:C	2:B:584:LEU:O	2.51	0.54
2:B:626:ASP:C	2:B:628:THR:N	2.62	0.54
1:A:160:PHE:CE1	1:A:166:LEU:HG	2.43	0.54
2:B:625:LEU:C	2:B:627:LEU:H	2.09	0.54
2:B:794:ARG:HA	2:B:795:ASP:C	2.34	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: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
2:B:522:GLN:NE2	2:B:529:GLU:CD	2.66	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
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
2:B:778:VAL:C	2:B:780:LYS:H	2.17	0.53
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
2:B:410:ARG:HH22	2:B:421:ILE:C	2.17	0.52
2:B:452:ARG:HH21	2:B:464:GLU:CD	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:211:GLY:HA3	1:C:295:PHE:CZ	2.44	0.52
1:C:284:GLY:C	1:C:285:ILE:HD12	2.35	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:C:238:ASP:CG	1:C:238:ASP:O	2.53	0.52
2:D:449:PRO:HD2	2:D:455:MET:CE	2.32	0.52
1:A:247:TYR:CE1	2:B:165:ASN:HB3	2.45	0.52
2:D:111:ARG:C	2:D:113:GLU:N	2.68	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: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:230:THR:HG23	2:B:234:MET:HE2	1.92	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:165:ASN:O	2:D:166:ARG:C	2.53	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:268:GLU:CD	4:C:999:AMP:H3'	2.34	0.51
1:C:322:PHE:O	1:C:325:GLN:HG2	2.10	0.51
2:D:43:HIS:O	2:D:97:ALA:HB1	2.09	0.51
2:D:54:ALA:O	2:D:55:GLN:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:705:ALA:HB2	2:D:763:GLN:CD	2.35	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:256:VAL:HG11	2:B:264:MET:HE2	1.91	0.51
2:D:319:GLY:C	2:D:321:HIS:N	2.64	0.51
2:B:140:ASP:CG	2:B:140:ASP:O	2.53	0.51
1:C:205:MET:HE1	2:D:512:THR:O	2.10	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
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
2:D:24:GLN:HG3	2:D:182:LEU:HD22	1.92	0.51
1:A:151:ALA:O	1:A:152:ARG:C	2.53	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: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:D:632:ASN:OD1	2:D:632:ASN:C	2.52	0.51
1:A:261:GLY:O	1:A:262:LYS:C	2.54	0.51
2:B:48:GLY:HA2	2:B:143:ILE:HG23	1.93	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
1:C:48:LEU:O	1:C:49:PRO:C	2.53	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:D:137:LEU:HB3	2:D:138:PRO:HD2	1.92	0.51
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
2:B:232:LEU:O	2:B:235:LYS:HB3	2.10	0.50
2:B:744:TYR:OH	2:B:747:LYS:N	2.44	0.50
2:D:731:GLY:HA2	2:D:735:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:614:PHE:CZ	1:C:94:VAL:HG22	2.46	0.50
1:C:107:HIS:ND1	1:C:107:HIS:C	2.69	0.50
2:D:441:LYS:HG2	2:D:441:LYS:O	2.09	0.50
1:A:178:MET:HE2	1:A:283:VAL:HG11	1.94	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
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:B:409:ARG:O	2:B:410:ARG:C	2.54	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:97:ALA:O	2:D:104:LYS:NZ	2.43	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:522:GLN:HE22	2:B:529:GLU:CD	2.17	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: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: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
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:230:THR:HG23	2:D:234:MET:HE2	1.94	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:591:MET:HE3	2:B:684:LEU:O	2.12	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
2:D:631:LEU:C	2:D:633:GLU:N	2.70	0.49
2:B:83:ASN:O	2:B:134:ILE:HD11	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:561:ASN:C	2:D:563:GLN:H	2.20	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
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:151:LEU:O	2:D:152:LYS:C	2.55	0.49
2:D:183:ASN:C	2:D:185:LEU:H	2.21	0.49
2:D:630:LYS:NZ	2:D:691:ASP:O	2.35	0.49
1:C:218:ILE:C	1:C:218:ILE:HD13	2.38	0.49
2:D:113:GLU:O	2:D:114:PRO:C	2.55	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:56:HIS:O	2:B:57:PRO:C	2.56	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:HG3	1:A:183:PRO:HD2	1.95	0.48
2:B:424:GLU:CD	2:B:424:GLU:H	2.21	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
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:570:PHE:CD1	2:B:570:PHE:C	2.91	0.48
2:B:631:LEU:CD2	2:B:632:ASN:N	2.77	0.48
2:B:696:GLN:O	2:B:697:ALA:C	2.56	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:666:HIS:CE1	2:B:668:GLU:OE2	2.67	0.48
2:B:774:ILE:C	2:B:776:ALA:N	2.71	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:289:LEU:C	2:D:291:ASP:H	2.22	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:174:GLN:HG3	1:A:212:LEU:HG	1.96	0.48
2:B:309:LYS:HZ1	2:B:321:HIS:CE1	2.31	0.48
2:B:344:THR:O	2:B:345:GLY:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:145:ILE:CG2	1:A:146:PRO:CA	2.91	0.48
2:B:703:PHE:O	2:B:763:GLN:NE2	2.47	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:101:ILE:O	1:C:102:GLU:C	2.57	0.47
2:D:565:ASN:O	2:D:565:ASN:CG	2.57	0.47
2:D:673:LEU:O	2:D:674:ASP:C	2.56	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
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:184:GLN:HA	2:D:432:ARG:NH1	2.29	0.47
1:A:218:ILE:HD12	1:A:218:ILE:C	2.39	0.47
2:B:134:ILE:HD12	2:B:134:ILE:H	1.80	0.47
2:B:138:PRO:O	2:B:139:ALA:C	2.58	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:411:SER:O	2:D:412:LYS:C	2.56	0.47
2:D:605:TRP:CZ3	2:D:606:ASN:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:HG13	1:A:186:ARG:N	2.30	0.47
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
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: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
1:A:276:HIS:CD2	1:A:278:ASN:HB2	2.50	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
1:C:154:ASP:C	1:C:156:ASP:H	2.23	0.47
2:D:38:VAL:HG13	2:D:155:ASP:O	2.15	0.47
2:D:536:PRO:C	2:D:538:SER:H	2.23	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
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: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
1:A:178:MET:HE1	1:A:280:LEU:HD23	1.97	0.46
2:B:230:THR:HG22	2:B:235:LYS:HB2	1.96	0.46
1:C:60:ILE:CG2	1:C:61:ASN:N	2.34	0.46
2:D:107:ALA:HA	2:D:116:GLU:HB3	1.98	0.46
2:D:229:PRO:O	2:D:230:THR:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:699:GLU:OE1	2:D:699:GLU:CA	2.62	0.46
2:B:231:PRO:O	2:B:232:LEU:C	2.59	0.46
2:B:520:VAL:O	2:B:521:GLN:C	2.58	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:53:CYS:O	2:D:54:ALA:C	2.58	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:53:CYS:C	2:D:54:ALA:O	2.57	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:172:ILE:O	2:B:173:ILE:C	2.57	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
2:D:512:THR:HB	2:D:571:GLU:CD	2.41	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:76:ALA:O	1:C:80:SER:OG	2.32	0.46
1:C:83:LEU:O	1:C:87:LEU:HG	2.14	0.46
1:C:304:MET:HE3	1:C:310:THR:O	2.16	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: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:790:GLN:CD	2:B:791:ALA:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLN:C	1:C:19:SER:N	2.74	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
2:B:183:ASN:O	2:B:184:GLN:HG2	2.17	0.45
1:C:260:MET:HE2	1:C:260:MET:HB3	1.89	0.45
2:B:73:ARG:HG3	2:B:73:ARG:HH11	1.81	0.45
2:B:276:ILE:O	2:B:276:ILE:HG22	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
2:D:682:PHE:C	2:D:682:PHE:CD2	2.94	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:D:673:LEU:C	2:D:674:ASP:O	2.60	0.45
1:A:295:PHE:C	1:A:295:PHE:CD2	2.94	0.45
2:B:123:SER:C	2:B:125:LEU:N	2.74	0.45
2:B:521:GLN:HE22	2:B:546:LEU:H	1.64	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
2:B:668:GLU:N	2:B:668:GLU:CD	2.74	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
1:C:71:LEU:C	1:C:73:ALA:N	2.72	0.45
1:C:216:THR:O	1:C:217:ASN:C	2.58	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: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:293:PHE:C	1:A:293:PHE:CD2	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:731:GLY:O	2:D:732:VAL:HG12	2.16	0.44
2:B:101:GLY:C	2:B:103:PHE:H	2.25	0.44
2:B:518:PRO:HG3	2:B:543:ALA:HB2	1.99	0.44
1:C:143:LEU:HD22	1:C:250:PHE:CD2	2.53	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
2:D:462:VAL:O	2:D:463:GLU:C	2.59	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: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:C:300:GLU:HB2	1:C:315:PHE:CE1	2.53	0.44
2:D:348:ARG:O	2:D:349:ARG:C	2.60	0.44
2:B:731:GLY:O	2:B:733:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLU:O	1:C:63:ALA:C	2.60	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:625:LEU:HD13	2:B:634:VAL:CG1	2.48	0.43
2:D:26:THR:CG2	2:D:32:VAL:HG22	2.48	0.43
2:D:599:ASN:O	2:D:600:ARG:C	2.61	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
2:B:142:PRO:O	2:B:143:ILE:C	2.61	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: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:269:LYS:C	2:B:271:ARG:H	2.26	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: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
1:C:150:PRO:O	1:C:151:ALA:C	2.61	0.43
2:D:1:MET:HB2	2:D:2:LYS:H	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:746:GLY:O	2:D:747:LYS:C	2.61	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:557:VAL:O	2:B:558:TYR:C	2.59	0.43
2:D:294:GLU:N	2:D:294:GLU:CD	2.76	0.43
2:D:471:TYR:O	2:D:472:ASN:C	2.61	0.43
2:D:536:PRO:HB2	2:D:537:ILE:HD12	2.01	0.43
2:D:565:ASN:CG	2:D:676:ASN:HD21	2.26	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
2:D:431:ARG:CZ	2:D:437:VAL:HG23	2.48	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:B:781:CYS:C	2:B:783:GLU:N	2.77	0.43
2:D:4:SER:O	2:D:5:GLU:C	2.61	0.43
2:D:294:GLU:CD	2:D:294:GLU:H	2.26	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:21:LEU:O	2:B:22:ALA:C	2.61	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:278:ASN:O	1:A:282:ASN:CG	2.62	0.42
2:B:113:GLU:HB2	2:B:114:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ASP:OD1	2:B:293:THR:HG22	2.19	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: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
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:338:PHE:HB2	2:B:343:ILE:HD11	2.00	0.42
1:C:75:LYS:O	1:C:75:LYS:CG	2.51	0.42
1:C:220:PHE:O	1:C:221:THR:C	2.63	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:142:PRO:C	2:D:144:GLY:N	2.78	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:43:HIS:ND1	2:B:43:HIS:C	2.77	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:O	2:B:566:ARG:HG2	2.18	0.42
2:B:567:VAL:HG23	2:B:569:ILE:HG23	2.00	0.42
1:C:154:ASP:C	1:C:156:ASP:N	2.77	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
1:A:186:ARG:C	1:A:187:ILE:HG23	2.45	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
2:D:396:ASN:O	2:D:397:GLU:C	2.62	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:32:LEU:C	1:C:34:LYS:H	2.28	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:346:ARG:O	2:D:347:ALA:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:106:LYS:O	2:B:107:ALA:C	2.61	0.41
2:B:311:LEU:HB2	2:B:322:SER:OG	2.20	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:165:ASN:H	2:B:165:ASN:ND2	2.01	0.41
2:B:209:ALA:H	2:B:210:PRO:CD	2.32	0.41
2:B:225:ASN:C	2:B:227:LYS:H	2.28	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: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:7:TRP:CD1	2:B:7:TRP:C	2.97	0.41
2:B:705:ALA:HB2	2:B:763:GLN:CD	2.46	0.41
2:B:790:GLN:HG3	2:B:791:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:GLY:H	2:D:346:ARG:NH1	2.12	0.41
2:D:597:CYS:HB2	2:D:679:THR:HG22	2.03	0.41
2:D:629:GLY:C	2:D:630:LYS:HG2	2.45	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
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
1:A:299:MET:HE2	1:A:299:MET:CA	2.45	0.41
2:B:163:THR:HA	2:B:164:PRO:HD3	1.91	0.41
1:C:65:GLU:CA	1:C:66:GLN:C	2.93	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:B:747:LYS:O	2:B:747:LYS:HG2	2.20	0.41
2:B:774:ILE:C	2:B:776:ALA:H	2.27	0.41
2:D:278:VAL:O	2:D:278:VAL:HG12	2.19	0.41
1:A:145:ILE:HB	1:A:146:PRO:C	2.45	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
1:A:209:MET:HE2	1:A:209:MET:HB2	1.95	0.41
2:B:67:VAL:HG22	2:B:77:ILE:HD12	2.03	0.41
2:B:151:LEU:C	2:B:152:LYS:HG2	2.46	0.41
2:B:288:VAL:O	2:B:320:GLU:N	2.54	0.41
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.90	0.41
1:C:124:GLY:O	1:C:125:PHE:C	2.64	0.41
2:D:644:LEU:HD22	2:D:663:GLY:HA3	2.03	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:B:452:ARG:NH2	2:B:464:GLU:CD	2.78	0.40
2:D:158:ILE:C	2:D:158:ILE:HD12	2.46	0.40
1:A:99:ARG:NH2	2:B:606:ASN:OD1	2.55	0.40
1:A:169:GLN:C	1:A:171:SER:H	2.29	0.40
2:B:89:ARG:HG2	2:B:141:ALA:HB3	2.02	0.40
2:B:641:ASN:C	2:B:641:ASN:HD22	2.29	0.40
2:B:783:GLU:C	2:B:785:LEU:N	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:300:GLU:CD	1:C:300:GLU:N	2.78	0.40
2:D:428:ASP:O	2:D:429:ILE:C	2.64	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: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: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
2:B:121:SER:H	2:B:124:GLU:CG	2.35	0.40
2:B:256:VAL:CG1	2:B:264:MET:HE2	2.52	0.40
2:B:280:MET:O	2:B:281:ALA:HB2	2.20	0.40
2:B:514:SER:O	2:B:545:ARG:HD2	2.22	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:238:ASP:C	1:C:239:LEU:O	2.65	0.40
2:D:230:THR:CG2	2:D:234:MET:HE2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/327 (73%)	197 (82%)	31 (13%)	12 (5%)	1	9
1	C	321/327 (98%)	231 (72%)	57 (18%)	33 (10%)	0	2
2	B	793/795 (100%)	631 (80%)	120 (15%)	42 (5%)	1	8
2	D	793/795 (100%)	628 (79%)	106 (13%)	59 (7%)	1	4
All	All	2147/2244 (96%)	1687 (79%)	314 (15%)	146 (7%)	1	4

All (146) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	187 (78%)	53 (22%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	656/663 (99%)	474 (72%)	182 (28%)	0	2
2	D	657/663 (99%)	480 (73%)	177 (27%)	0	2
All	All	1765/1878 (94%)	1305 (74%)	460 (26%)	0	3

All (460) 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
1	A	101	ILE
1	A	103	ASN
1	A	106	LEU
1	A	109	VAL
1	A	113	ILE
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	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	257	VAL
1	A	263	ASN

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Mol	Chain	Res	Type
1	A	265	LYS
1	A	268	GLU
1	A	269	VAL
1	A	282	ASN
1	A	283	VAL
1	A	288	GLU
1	A	301	ARG
1	A	302	LEU
1	A	305	LEU
1	A	310	THR
1	A	317	GLU
1	A	320	LEU
1	A	323	LEU
1	A	324	LYS
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	43	HIS
2	B	52	GLU
2	B	53	CYS
2	B	61	LYS
2	B	62	LEU
2	B	73	ARG
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	90	VAL
2	B	92	VAL
2	B	103	PHE
2	B	104	LYS
2	B	106	LYS
2	B	109	LYS

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Mol	Chain	Res	Type
2	B	111	ARG
2	B	113	GLU
2	B	124	GLU
2	B	127	ILE
2	B	128	SER
2	B	131	HIS
2	B	134	ILE
2	B	137	LEU
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
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	224	ILE
2	B	225	ASN
2	B	227	LYS
2	B	230	THR
2	B	235	LYS
2	B	244	ARG
2	B	246	ILE
2	B	249	VAL
2	B	257	LEU
2	B	269	LYS
2	B	272	ILE
2	B	276	ILE
2	B	285	GLU
2	B	288	VAL
2	B	293	THR
2	B	294	GLU

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Mol	Chain	Res	Type
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	362	ARG
2	B	364	VAL
2	B	370	HIS
2	B	371	LYS
2	B	374	GLU
2	B	375	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
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	439	GLU
2	B	445	GLN
2	B	447	VAL
2	B	452	ARG
2	B	457	ILE
2	B	468	VAL
2	B	472	ASN
2	B	473	ASN
2	B	476	ASP
2	B	479	VAL

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Mol	Chain	Res	Type
2	B	487	THR
2	B	493	LEU
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	577	VAL
2	B	584	LEU
2	B	586	ILE
2	B	590	LEU
2	B	595	VAL
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	634	VAL
2	B	641	ASN
2	B	659	ILE
2	B	662	VAL
2	B	664	VAL
2	B	665	VAL
2	B	667	PRO
2	B	668	GLU
2	B	671	ARG

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Mol	Chain	Res	Type
2	B	676	ASN
2	B	678	ARG
2	B	685	GLU
2	B	688	LYS
2	B	700	ILE
2	B	714	VAL
2	B	716	GLU
2	B	724	LEU
2	B	728	LYS
2	B	730	VAL
2	B	732	VAL
2	B	733	ASN
2	B	734	GLN
2	B	735	VAL
2	B	738	VAL
2	B	739	ASN
2	B	740	LEU
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	778	VAL
2	B	780	LYS
2	B	787	GLU
2	B	788	ARG
1	C	21	VAL
1	C	30	GLU
1	C	62	GLU
1	C	65	GLU
1	C	69	GLN
1	C	71	LEU
1	C	72	ASN
1	C	74	ARG
1	C	75	LYS
1	C	83	LEU
1	C	91	THR
1	C	94	VAL
1	C	96	LEU
1	C	101	ILE

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Mol	Chain	Res	Type
1	C	103	ASN
1	C	106	LEU
1	C	109	VAL
1	C	111	ARG
1	C	112	THR
1	C	113	ILE
1	C	115	ARG
1	C	122	GLU
1	C	123	LEU
1	C	126	THR
1	C	145	ILE
1	C	155	HIS
1	C	164	ARG
1	C	165	LEU
1	C	173	VAL
1	C	181	GLN
1	C	185	ILE
1	C	201	THR
1	C	203	THR
1	C	209	MET
1	C	213	ILE
1	C	218	ILE
1	C	238	ASP
1	C	239	LEU
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	289	VAL
1	C	291	SER
1	C	300	GLU
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	16	ILE
2	D	18	SER

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Mol	Chain	Res	Type
2	D	19	ASP
2	D	21	LEU
2	D	30	LEU
2	D	35	VAL
2	D	36	GLU
2	D	47	VAL
2	D	50	VAL
2	D	52	GLU
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	74	LEU
2	D	77	ILE
2	D	92	VAL
2	D	95	ILE
2	D	104	LYS
2	D	110	LEU
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	147	ILE
2	D	152	LYS
2	D	158	ILE
2	D	161	SER
2	D	164	PRO
2	D	165	ASN
2	D	172	ILE
2	D	181	VAL
2	D	182	LEU
2	D	188	VAL
2	D	195	VAL
2	D	198	THR
2	D	199	ILE
2	D	201	ASP

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Mol	Chain	Res	Type
2	D	202	THR
2	D	203	LEU
2	D	211	GLU
2	D	222	LYS
2	D	224	ILE
2	D	226	VAL
2	D	227	LYS
2	D	234	MET
2	D	238	LEU
2	D	244	ARG
2	D	272	ILE
2	D	273	GLU
2	D	276	ILE
2	D	277	VAL
2	D	278	VAL
2	D	279	ARG
2	D	280	MET
2	D	282	LYS
2	D	287	LEU
2	D	290	LEU
2	D	294	GLU
2	D	296	LYS
2	D	302	LEU
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	329	GLN
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	383	ILE
2	D	387	GLU
2	D	392	ILE
2	D	394	ILE

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Mol	Chain	Res	Type
2	D	395	THR
2	D	396	ASN
2	D	400	LEU
2	D	402	LYS
2	D	403	ARG
2	D	406	ILE
2	D	407	THR
2	D	408	LEU
2	D	426	VAL
2	D	427	THR
2	D	430	LEU
2	D	437	VAL
2	D	438	THR
2	D	439	GLU
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
2	D	512	THR
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	539	VAL
2	D	546	LEU
2	D	556	VAL
2	D	559	ASN
2	D	560	GLN
2	D	564	GLN
2	D	566	ARG
2	D	574	LEU
2	D	577	VAL
2	D	584	LEU
2	D	586	ILE

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Mol	Chain	Res	Type
2	D	590	LEU
2	D	592	LEU
2	D	595	VAL
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	627	LEU
2	D	628	THR
2	D	630	LYS
2	D	631	LEU
2	D	632	ASN
2	D	639	GLU
2	D	644	LEU
2	D	657	GLU
2	D	664	VAL
2	D	665	VAL
2	D	668	GLU
2	D	674	ASP
2	D	678	ARG
2	D	688	LYS
2	D	689	LEU
2	D	691	ASP
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	724	LEU
2	D	732	VAL
2	D	735	VAL
2	D	740	LEU
2	D	758	ILE
2	D	760	LEU
2	D	761	ILE
2	D	762	LEU
2	D	767	ARG
2	D	768	THR
2	D	771	GLU

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Mol	Chain	Res	Type
2	D	774	ILE
2	D	778	VAL
2	D	783	GLU
2	D	786	LYS
2	D	787	GLU
2	D	790	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) 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	278	ASN
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	254	ASN
2	B	262	GLN
2	B	265	HIS
2	B	321	HIS
2	B	350	HIS
2	B	369	GLN
2	B	370	HIS
2	B	396	ASN
2	B	420	HIS
2	B	425	GLN
2	B	472	ASN
2	B	521	GLN
2	B	522	GLN
2	B	525	HIS

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Mol	Chain	Res	Type
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	207	HIS
1	C	208	GLN
1	C	222	ASN
1	C	276	HIS
1	C	325	GLN
2	D	23	ASN
2	D	56	HIS
2	D	58	ASN
2	D	156	ASN
2	D	165	ASN
2	D	225	ASN
2	D	254	ASN
2	D	321	HIS
2	D	369	GLN
2	D	445	GLN
2	D	473	ASN
2	D	480	GLN
2	D	521	GLN
2	D	525	HIS
2	D	563	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	980	-	11,12,12	0.73	0	11,15,15	0.46	0
3	PHE	C	990	-	11,12,12	0.78	0	11,15,15	0.86	1 (9%)
4	AMP	A	992	-	25,25,25	1.65	5 (20%)	37,38,38	1.84	9 (24%)
4	AMP	C	999	-	25,25,25	1.44	3 (12%)	37,38,38	1.91	8 (21%)

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	A	980	-	-	3/8/8/8	0/1/1/1
3	PHE	C	990	-	-	4/8/8/8	0/1/1/1
4	AMP	A	992	-	-	7/10/26/26	0/3/3/3
4	AMP	C	999	-	-	7/10/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	992	AMP	P-O1P	4.35	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	999	AMP	P-O1P	4.25	1.63	1.50
4	A	992	AMP	C5-N7	-3.71	1.32	1.39
4	C	999	AMP	C5-N7	-2.99	1.33	1.39
4	A	992	AMP	C1'-N9	2.70	1.53	1.46
4	A	992	AMP	C4-N9	-2.49	1.32	1.37
4	C	999	AMP	C1'-N9	2.16	1.52	1.46
4	A	992	AMP	P-O3P	2.12	1.62	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	999	AMP	C5-C4-N3	-5.48	119.17	126.72
4	A	992	AMP	N3-C2-N1	-4.92	121.14	128.58
4	C	999	AMP	N3-C2-N1	-4.73	121.42	128.58
4	C	999	AMP	N3-C4-N9	4.07	134.08	127.17
4	A	992	AMP	O4'-C1'-C2'	-3.84	98.40	106.62
4	A	992	AMP	C5-C4-N3	-3.70	121.63	126.72
4	C	999	AMP	C2-N3-C4	3.67	120.79	111.83
4	A	992	AMP	O2P-P-O5'	3.25	115.13	106.67
4	C	999	AMP	N9-C8-N7	-2.81	109.94	113.94
4	A	992	AMP	C2-N3-C4	2.77	118.60	111.83
3	C	990	PHE	OXT-C-O	-2.69	117.97	124.08
4	A	992	AMP	N3-C4-N9	2.66	131.68	127.17
4	C	999	AMP	C5-N7-C8	2.57	107.49	103.45
4	A	992	AMP	O3P-P-O5'	-2.55	100.01	106.67
4	A	992	AMP	N9-C8-N7	-2.21	110.81	113.94
4	A	992	AMP	C2-N1-C6	2.20	122.34	118.73
4	C	999	AMP	C4-C5-N7	-2.09	108.19	110.58
4	C	999	AMP	C2'-C1'-N9	2.05	118.39	113.30

There are no chirality outliers.

All (21) 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'

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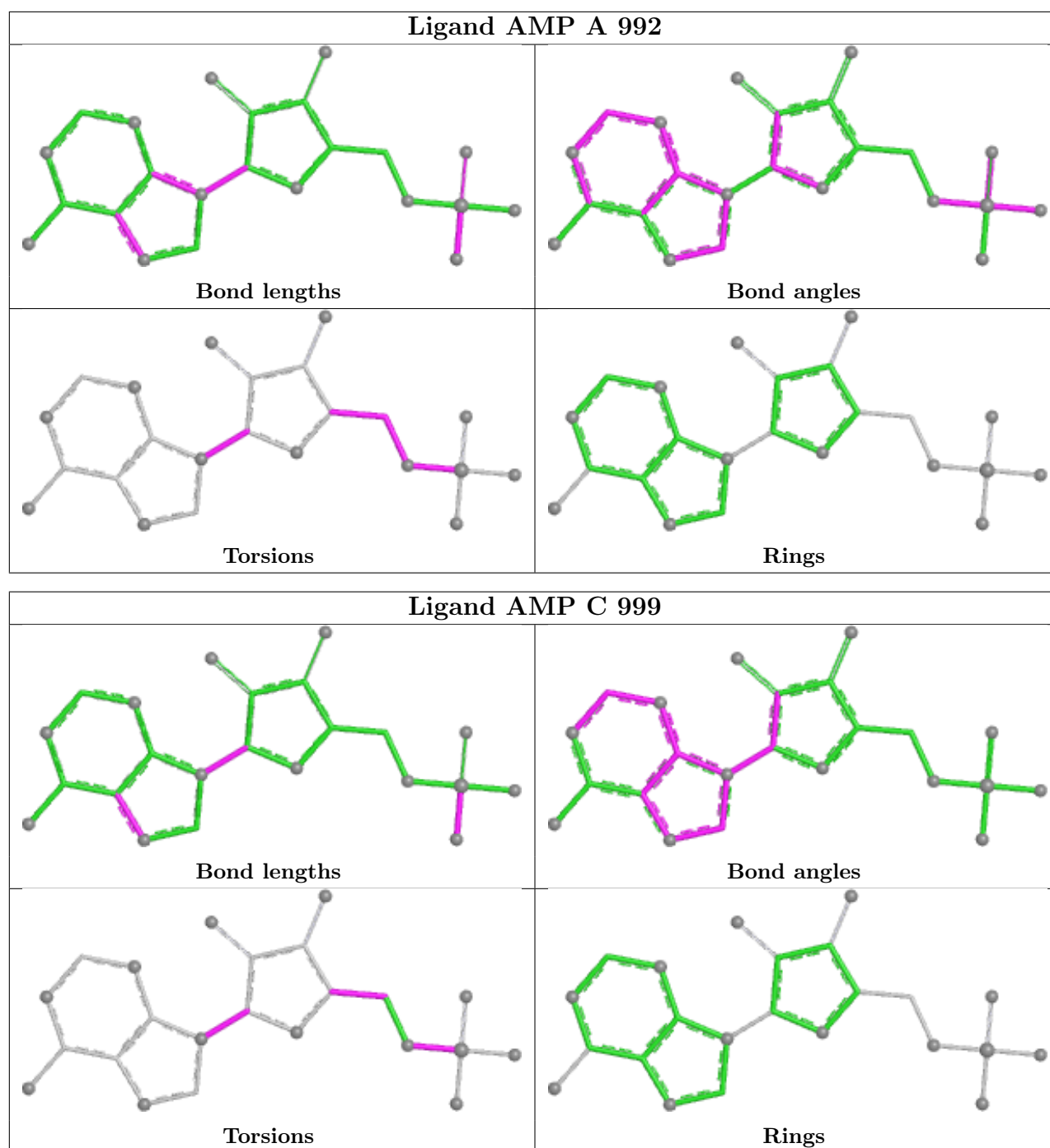
Mol	Chain	Res	Type	Atoms
4	C	999	AMP	C3'-C4'-C5'-O5'
4	C	999	AMP	C2'-C1'-N9-C4
4	A	992	AMP	O4'-C4'-C5'-O5'
4	C	999	AMP	C2'-C1'-N9-C8
4	A	992	AMP	C2'-C1'-N9-C4
4	A	992	AMP	C3'-C4'-C5'-O5'
4	A	992	AMP	C2'-C1'-N9-C8
3	A	980	PHE	CA-CB-CG-CD2
3	A	980	PHE	CA-CB-CG-CD1
3	C	990	PHE	OXT-C-CA-CB
3	C	990	PHE	O-C-CA-CB
4	A	992	AMP	C4'-C5'-O5'-P
3	A	980	PHE	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	980	PHE	2	0
3	C	990	PHE	1	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	242/327 (74%)	0.23	8 (3%)	49	28	50, 63, 87, 145	0
1	C	323/327 (98%)	0.81	25 (7%)	19	10	36, 89, 164, 169	8 (2%)
2	B	795/795 (100%)	0.31	8 (1%)	79	59	51, 89, 128, 148	0
2	D	795/795 (100%)	0.74	43 (5%)	31	16	58, 97, 132, 148	0
All	All	2155/2244 (96%)	0.53	84 (3%)	43	24	36, 90, 136, 169	8 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	23	ALA	8.7
1	C	19	SER	5.6
2	D	345	GLY	4.3
1	C	243	PHE	4.3
1	C	18	ALA	3.9
1	C	29	VAL	3.8
2	D	114	PRO	3.8
1	C	22	ALA	3.7
1	C	32	LEU	3.6
2	D	794	ARG	3.6
2	D	261	GLY	3.6
2	D	169	CYS	3.6
1	C	261	GLY	3.5
1	C	20	ASP	3.3
2	D	81	ALA	3.2
1	C	25	ASP	3.2
2	D	84	CYS	3.2
2	D	88	LEU	3.2
2	B	79	CYS	3.0
1	C	21	VAL	3.0
2	B	626	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	781	CYS	2.7
2	D	78	VAL	2.7
2	D	82	PRO	2.7
2	D	211	GLU	2.7
2	D	91	ALA	2.7
2	D	120	CYS	2.7
1	C	24	LEU	2.7
1	A	196	ASN	2.7
1	C	14	ALA	2.6
2	D	294	GLU	2.6
2	D	281	ALA	2.6
1	C	26	ASN	2.5
2	D	795	ASP	2.5
2	D	95	ILE	2.5
2	D	143	ILE	2.5
2	B	444	TRP	2.5
2	D	546	LEU	2.5
2	D	29	GLY	2.5
1	A	264	GLY	2.4
2	D	714	VAL	2.4
2	D	113	GLU	2.4
1	C	44	THR	2.4
2	D	175	VAL	2.4
2	D	466	ALA	2.4
1	C	267	LEU	2.4
2	D	221	VAL	2.4
2	D	201	ASP	2.3
1	A	87	LEU	2.3
1	C	38	LEU	2.3
2	D	136	GLU	2.3
2	D	634	VAL	2.3
1	C	148	HIS	2.3
1	C	155	HIS	2.3
2	B	62	LEU	2.3
2	D	266	ALA	2.3
2	D	163	THR	2.3
2	D	115	SER	2.3
2	D	267	PHE	2.3
1	A	188	ILE	2.2
2	D	216	TYR	2.2
1	A	136	ASP	2.2
2	D	394	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	152	LYS	2.2
1	A	195	ARG	2.2
1	C	239	LEU	2.1
2	D	455	MET	2.1
2	B	730	VAL	2.1
2	B	721	ALA	2.1
2	D	631	LEU	2.1
1	C	49	PRO	2.1
1	C	28	ARG	2.1
1	A	304	MET	2.1
1	C	27	VAL	2.1
2	D	426	VAL	2.1
1	A	145	ILE	2.1
2	D	94	THR	2.1
1	C	31	TYR	2.0
1	C	39	THR	2.0
2	D	79	CYS	2.0
2	B	138	PRO	2.0
2	D	135	ILE	2.0
2	D	541	MET	2.0
2	D	433	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AMP	C	999	23/23	0.78	0.16	137,145,147,147	0
4	AMP	A	992	23/23	0.90	0.14	96,99,101,101	0

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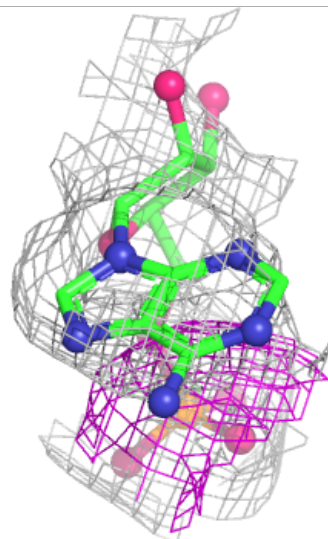
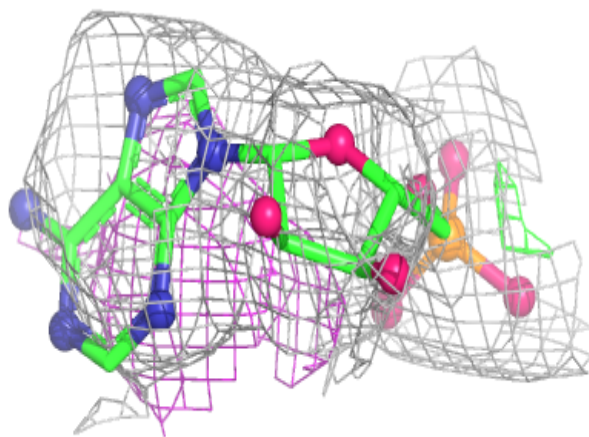
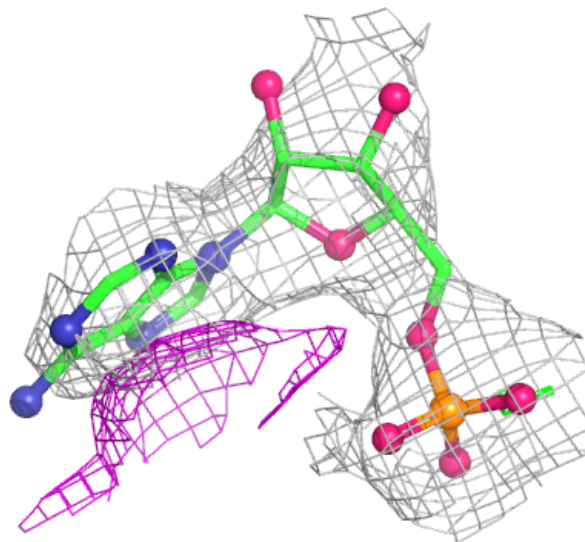
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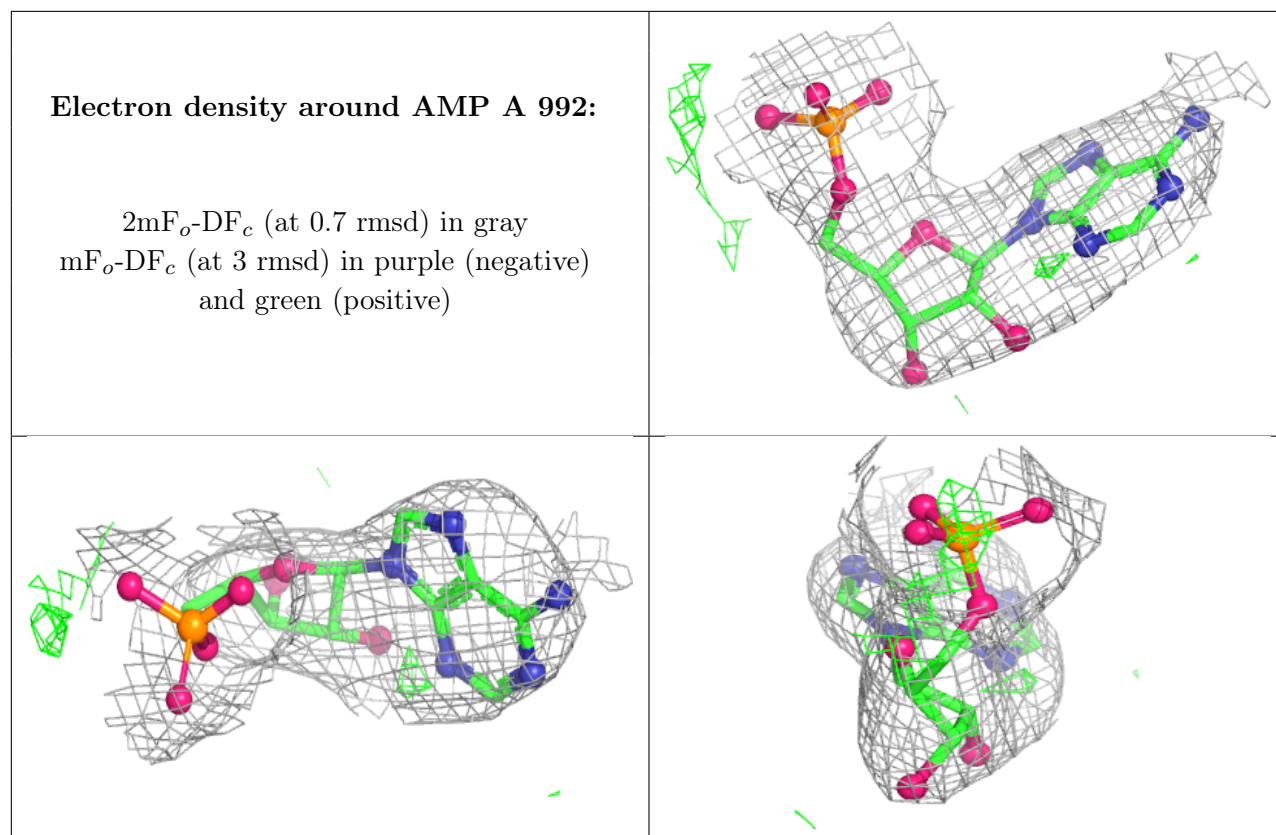
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PHE	A	980	12/12	0.91	0.20	73,80,87,87	0
3	PHE	C	990	12/12	0.91	0.16	95,98,99,99	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.