



wwPDB EM Map/Model Validation Report ⓘ

May 5, 2016 – 05:30 PM EDT

PDB ID : 4CRN
EMDB ID: : EMD-2597
Title : Cryo-EM of a pretermination complex with eRF1 and eRF3
Authors : Preis, A.; Heuer, A.; Barrio-Garcia, C.; Hauser, A.; Eyler, D.; Berninghausen, O.; Green, R.; Becker, T.; Beckmann, R.
Deposited on : 2014-02-28
Resolution : 9.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

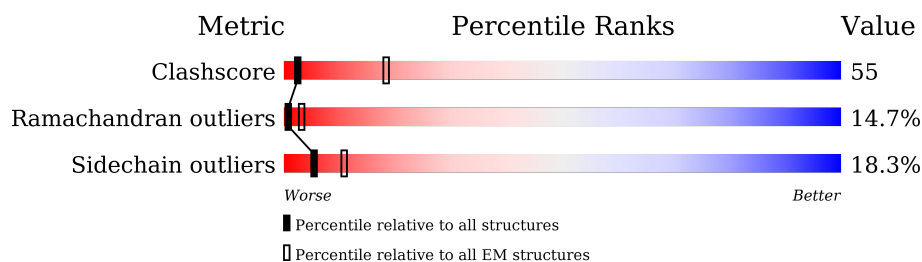
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	P	430	
2	X	437	

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
3	GNP	P	1685	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6693 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ERF3 IN RIBOSOME BOUND ERF1-ERF3-GDPNP COMPLEX.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	430	Total	C	N	O	S	0	0
			3351	2119	577	634	21		

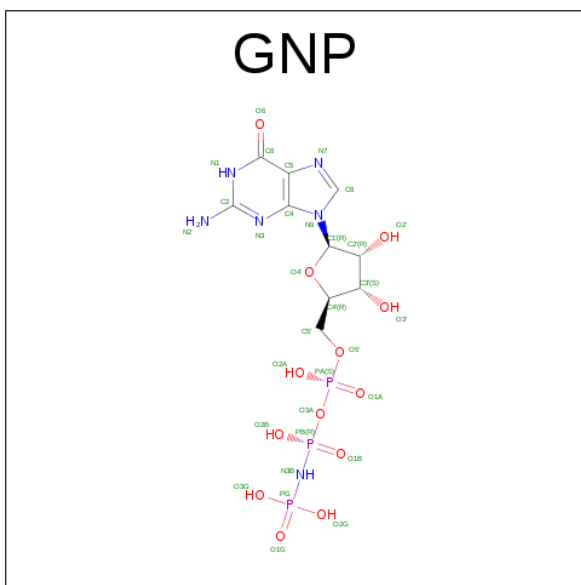
- Molecule 2 is a protein called ERF1 IN RIBOSOME-BOUND ERF1-ERF3-GDPNP COMPLEX.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	422	Total	C	N	O	S	0	1
			3310	2110	548	642	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	41	LEU	GLN	CONFLICT	UNP P12385
X	300	PHE	TYR	CONFLICT	UNP P12385

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

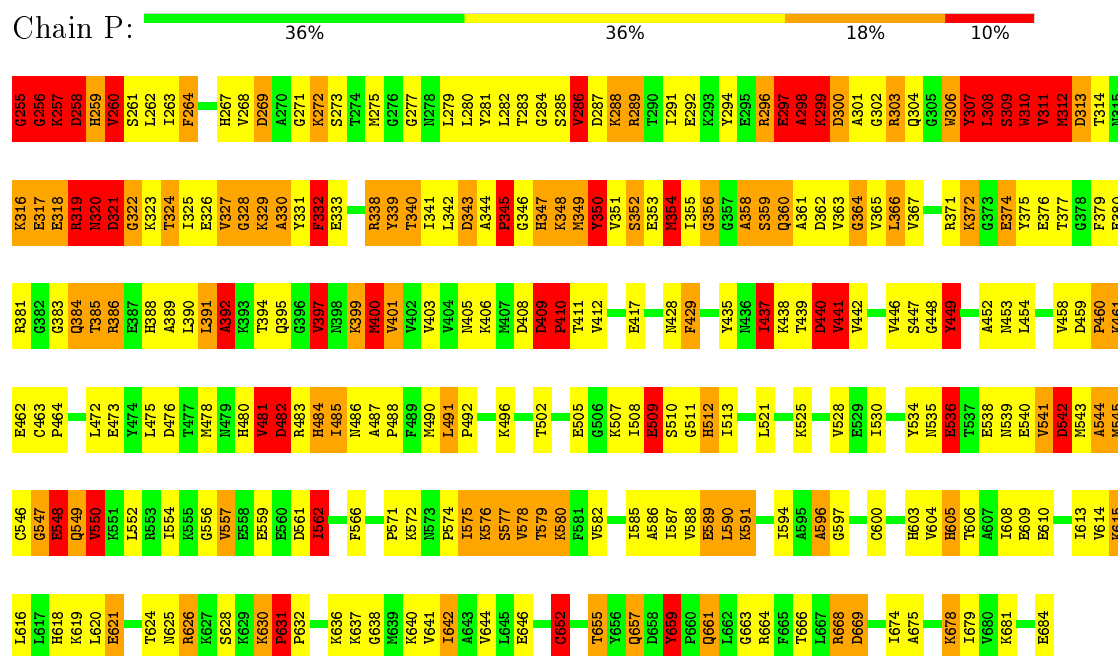


Mol	Chain	Residues	Atoms					AltConf
3	P	1	Total	C	N	O	P	0
			32	10	6	13	3	

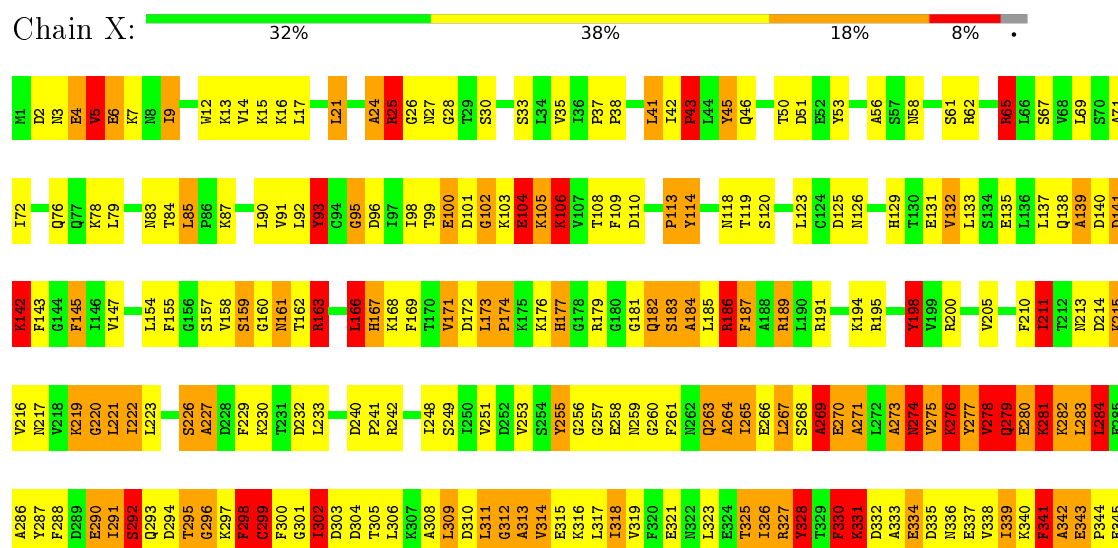
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: ERF3 IN RIBOSOME BOUND ERF1-ERF3-GDPNP COMPLEX



• Molecule 2: ERF1 IN RIBOSOME-BOUND ERF1-ERF3-GDPNP COMPLEX






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.02	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	TEMCAM F416 CMOS TVIPS	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP

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 >2	RMSZ	# Z >2
1	P	0.96	6/3412 (0.2%)	1.77	88/4600 (1.9%)
2	X	1.94	17/3363 (0.5%)	2.21	148/4532 (3.3%)
All	All	1.53	23/6775 (0.3%)	2.00	236/9132 (2.6%)

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	P	0	95
2	X	1	25
All	All	1	120

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	379	ASN	CG-ND2	81.72	3.37	1.32
2	X	183	SER	C-N	22.62	1.86	1.34
2	X	182	GLN	C-N	16.32	1.71	1.34
2	X	421	SER	C-N	-14.59	1.00	1.34
1	P	330	ALA	C-N	13.98	1.66	1.34
1	P	684	GLU	C-O	-12.07	1.00	1.23
2	X	421	SER	C-O	-12.07	1.00	1.23
2	X	269	ALA	C-N	-10.46	1.09	1.34
2	X	342	ALA	C-N	8.84	1.54	1.34
2	X	368	PRO	CA-C	8.31	1.69	1.52
1	P	356	GLY	CA-C	-6.93	1.40	1.51
1	P	409	ASP	CG-OD1	-6.89	1.09	1.25
2	X	368	PRO	C-N	5.99	1.47	1.34
2	X	95	GLY	CA-C	-5.96	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	256	GLY	CA-C	5.67	1.60	1.51
2	X	174	PRO	N-CA	5.47	1.56	1.47
2	X	269	ALA	N-CA	5.46	1.57	1.46
2	X	368	PRO	N-CA	5.21	1.56	1.47
2	X	342	ALA	N-CA	-5.21	1.35	1.46
2	X	62	ARG	CD-NE	5.18	1.55	1.46
2	X	37	PRO	CA-C	-5.16	1.42	1.52
1	P	259	HIS	CB-CG	5.12	1.59	1.50
2	X	109	PHE	CG-CD1	5.04	1.46	1.38

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	379	ASN	OD1-CG-ND2	-44.57	19.39	121.90
2	X	269	ALA	O-C-N	-24.66	83.25	122.70
2	X	183	SER	O-C-N	23.00	159.49	122.70
1	P	545	MET	CG-SD-CE	21.25	134.19	100.20
2	X	183	SER	CA-C-N	-17.73	78.19	117.20
2	X	93	TYR	CB-CG-CD1	14.70	129.82	121.00
1	P	350	TYR	CB-CG-CD2	-14.51	112.29	121.00
2	X	51	ASP	CB-CG-OD2	-14.51	105.24	118.30
2	X	173	LEU	O-C-N	-14.33	93.88	121.10
1	P	320	ASN	C-N-CA	13.84	156.31	121.70
2	X	51	ASP	CB-CG-OD1	13.44	130.40	118.30
2	X	195	ARG	NE-CZ-NH1	12.80	126.70	120.30
2	X	93	TYR	CB-CG-CD2	-12.47	113.52	121.00
2	X	183	SER	C-N-CA	-12.46	90.55	121.70
2	X	341	PHE	CB-CG-CD1	12.34	129.44	120.80
2	X	189	ARG	NE-CZ-NH1	12.12	126.36	120.30
2	X	421	SER	O-C-N	12.05	141.99	122.70
1	P	321	ASP	N-CA-C	11.92	143.19	111.00
1	P	545	MET	CA-CB-CG	11.61	133.03	113.30
1	P	350	TYR	CG-CD2-CE2	-11.56	112.05	121.30
2	X	369	LEU	CB-CA-C	-11.41	88.51	110.20
1	P	321	ASP	CB-CA-C	-11.35	87.69	110.40
2	X	142	LYS	N-CA-CB	11.17	130.71	110.60
2	X	210	PHE	CB-CG-CD1	-11.14	113.00	120.80
2	X	114	TYR	CB-CG-CD1	-11.00	114.40	121.00
2	X	367	GLU	CA-C-N	10.65	146.91	117.10
2	X	173	LEU	CA-C-N	10.39	146.19	117.10
2	X	15	LYS	CB-CA-C	10.32	131.03	110.40
2	X	328	TYR	CB-CG-CD2	-10.23	114.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	330	ALA	O-C-N	10.17	138.97	122.70
2	X	341	PHE	CB-CG-CD2	-10.12	113.71	120.80
1	P	400	MET	CB-CA-C	9.93	130.26	110.40
2	X	341	PHE	N-CA-CB	9.87	128.37	110.60
2	X	198	TYR	CB-CG-CD2	-9.76	115.14	121.00
2	X	366	GLU	C-N-CA	9.76	146.10	121.70
2	X	367	GLU	CA-C-O	-9.73	99.67	120.10
2	X	186	ARG	CB-CA-C	-9.64	91.12	110.40
1	P	321	ASP	CB-CG-OD1	-9.60	109.66	118.30
2	X	291	ILE	CB-CA-C	-9.54	92.52	111.60
1	P	319	ARG	NE-CZ-NH1	-9.47	115.56	120.30
1	P	320	ASN	CA-C-N	-9.42	96.48	117.20
2	X	174	PRO	CB-CA-C	-9.29	88.77	112.00
2	X	342	ALA	CB-CA-C	9.18	123.86	110.10
1	P	316	LYS	CB-CA-C	-9.17	92.06	110.40
2	X	3	ASN	N-CA-C	-9.07	86.50	111.00
2	X	84	THR	N-CA-CB	9.01	127.42	110.30
2	X	281	LYS	C-N-CA	8.95	144.08	121.70
2	X	277	TYR	CB-CG-CD2	-8.80	115.72	121.00
2	X	331	LYS	N-CA-CB	8.65	126.17	110.60
1	P	379	PHE	C-N-CA	8.65	143.32	121.70
2	X	33	SER	N-CA-CB	8.55	123.33	110.50
1	P	318	GLU	O-C-N	-8.51	109.08	122.70
2	X	5	VAL	CB-CA-C	8.47	127.50	111.40
2	X	273	ALA	C-N-CA	8.47	142.88	121.70
1	P	348	LYS	CB-CA-C	-8.41	93.58	110.40
1	P	380	GLU	N-CA-C	-8.36	88.42	111.00
2	X	299	CYS	C-N-CA	8.34	142.54	121.70
2	X	174	PRO	CA-N-CD	-8.19	100.03	111.50
1	P	545	MET	CB-CA-C	-8.17	94.05	110.40
2	X	396	GLN	CB-CA-C	-8.15	94.11	110.40
2	X	24	ALA	N-CA-CB	8.09	121.43	110.10
2	X	177	HIS	CA-CB-CG	8.04	127.26	113.60
2	X	281	LYS	CB-CA-C	8.03	126.47	110.40
2	X	342	ALA	N-CA-CB	-8.00	98.91	110.10
1	P	481	VAL	CA-CB-CG2	8.00	122.89	110.90
2	X	284	LEU	CB-CA-C	-7.98	95.04	110.20
2	X	264	ALA	N-CA-CB	7.96	121.25	110.10
2	X	292	SER	O-C-N	-7.89	110.08	122.70
2	X	198	TYR	CB-CG-CD1	7.87	125.72	121.00
1	P	330	ALA	CA-C-N	-7.69	100.28	117.20
1	P	307	TYR	N-CA-CB	-7.64	96.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	182	GLN	C-N-CA	-7.62	102.65	121.70
1	P	397	VAL	CG1-CB-CG2	-7.48	98.93	110.90
1	P	338	ARG	N-CA-CB	7.47	124.05	110.60
2	X	137	LEU	N-CA-C	-7.46	90.85	111.00
2	X	227	ALA	N-CA-CB	-7.45	99.67	110.10
2	X	242	ARG	NE-CZ-NH1	7.45	124.02	120.30
2	X	226	SER	CB-CA-C	-7.38	96.08	110.10
2	X	139	ALA	N-CA-CB	7.38	120.42	110.10
2	X	182	GLN	CA-C-N	-7.35	101.04	117.20
2	X	369	LEU	N-CA-CB	7.35	125.09	110.40
2	X	298	PHE	CB-CG-CD1	7.28	125.89	120.80
2	X	220	GLY	N-CA-C	7.26	131.26	113.10
1	P	324	THR	CA-CB-CG2	-7.23	102.28	112.40
1	P	449	TYR	CZ-CE2-CD2	-7.22	113.30	119.80
1	P	400	MET	CA-CB-CG	7.17	125.49	113.30
2	X	85	LEU	N-CA-CB	-7.17	96.06	110.40
2	X	6	GLU	CB-CA-C	-7.14	96.13	110.40
1	P	321	ASP	N-CA-CB	-7.11	97.80	110.60
2	X	214	ASP	CB-CG-OD2	7.10	124.69	118.30
2	X	342	ALA	C-N-CA	-7.04	104.10	121.70
1	P	435	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	P	257	LYS	N-CA-CB	6.99	123.19	110.60
1	P	545	MET	N-CA-CB	6.98	123.17	110.60
2	X	279	GLN	N-CA-CB	6.97	123.15	110.60
2	X	405	GLY	O-C-N	-6.97	111.55	122.70
2	X	210	PHE	CB-CG-CD2	6.97	125.68	120.80
2	X	174	PRO	O-C-N	-6.95	111.58	122.70
2	X	177	HIS	C-N-CA	6.93	136.86	122.30
2	X	277	TYR	CB-CG-CD1	6.93	125.16	121.00
2	X	5	VAL	CG1-CB-CG2	-6.90	99.87	110.90
1	P	332	PHE	CB-CG-CD2	-6.89	115.98	120.80
2	X	290	GLU	CB-CA-C	6.87	124.14	110.40
2	X	177	HIS	CB-CA-C	-6.87	96.67	110.40
2	X	16	LYS	CB-CA-C	-6.85	96.70	110.40
1	P	255	GLY	CA-C-O	-6.84	108.28	120.60
1	P	321	ASP	CB-CG-OD2	6.84	124.46	118.30
1	P	289	ARG	NE-CZ-NH1	6.81	123.70	120.30
2	X	330	PHE	CB-CG-CD2	-6.79	116.05	120.80
1	P	332	PHE	CB-CG-CD1	6.74	125.52	120.80
2	X	83	ASN	CB-CA-C	6.70	123.80	110.40
1	P	482	ASP	CB-CG-OD1	-6.67	112.30	118.30
2	X	65	ARG	NE-CZ-NH1	-6.67	116.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	491	LEU	CB-CG-CD2	6.63	122.27	111.00
1	P	296	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	P	306	TRP	CB-CA-C	6.54	123.47	110.40
1	P	449	TYR	CB-CG-CD2	-6.50	117.10	121.00
2	X	273	ALA	N-CA-C	-6.49	93.47	111.00
2	X	219	LYS	CB-CA-C	6.46	123.32	110.40
2	X	110	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	P	562	ILE	CA-CB-CG1	6.44	123.23	111.00
2	X	25	ARG	C-N-CA	6.42	135.78	122.30
2	X	330	PHE	O-C-N	-6.38	112.49	122.70
1	P	303	ARG	N-CA-CB	-6.38	99.12	110.60
1	P	320	ASN	CB-CA-C	6.37	123.14	110.40
1	P	349	MET	CB-CA-C	-6.36	97.68	110.40
2	X	363	VAL	CA-CB-CG2	-6.36	101.37	110.90
1	P	320	ASN	O-C-N	6.34	132.84	122.70
2	X	110	ASP	CB-CG-OD1	6.34	124.00	118.30
2	X	265	ILE	CB-CA-C	-6.33	98.94	111.60
2	X	379	ASN	CB-CG-ND2	-6.33	101.52	116.70
1	P	299	LYS	CA-C-N	-6.31	103.31	117.20
2	X	364	VAL	CG1-CB-CG2	6.29	120.97	110.90
2	X	14	VAL	C-N-CA	6.27	137.37	121.70
2	X	17	LEU	CB-CG-CD1	6.26	121.64	111.00
1	P	317	GLU	N-CA-CB	6.26	121.87	110.60
1	P	350	TYR	CA-CB-CG	6.25	125.27	113.40
1	P	659	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	P	255	GLY	C-N-CA	6.19	135.29	122.30
2	X	4	GLU	N-CA-C	-6.04	94.69	111.00
2	X	187	PHE	CB-CG-CD2	-6.04	116.58	120.80
1	P	318	GLU	CA-C-N	5.99	130.39	117.20
1	P	286	VAL	CA-CB-CG2	5.98	119.86	110.90
2	X	84	THR	CB-CA-C	-5.98	95.46	111.60
1	P	257	LYS	CB-CG-CD	5.97	127.13	111.60
2	X	269	ALA	N-CA-C	5.97	127.11	111.00
1	P	354	MET	CA-CB-CG	5.95	123.42	113.30
2	X	9	ILE	N-CA-CB	5.94	124.47	110.80
2	X	84	THR	N-CA-C	-5.93	94.99	111.00
2	X	325	THR	N-CA-CB	5.89	121.50	110.30
2	X	41	LEU	N-CA-CB	5.86	122.12	110.40
2	X	211	ILE	CB-CA-C	5.86	123.31	111.60
1	P	259	HIS	CB-CA-C	5.82	122.05	110.40
2	X	349	LYS	N-CA-CB	5.82	121.08	110.60
1	P	578	VAL	C-N-CA	5.82	136.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	9	ILE	O-C-N	-5.82	113.40	122.70
2	X	276	LYS	N-CA-CB	-5.79	100.18	110.60
2	X	273	ALA	CA-C-N	-5.74	104.57	117.20
1	P	307	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	P	308	LEU	N-CA-C	5.74	126.49	111.00
2	X	172	ASP	N-CA-C	-5.73	95.52	111.00
2	X	56	ALA	CB-CA-C	5.72	118.68	110.10
1	P	302	GLY	C-N-CA	5.72	135.99	121.70
2	X	161	ASN	N-CA-C	-5.71	95.58	111.00
2	X	341	PHE	CA-CB-CG	5.70	127.57	113.90
1	P	441	VAL	N-CA-CB	5.69	124.01	111.50
2	X	341	PHE	CB-CA-C	-5.67	99.06	110.40
2	X	5	VAL	CA-CB-CG2	5.65	119.37	110.90
1	P	297	GLU	C-N-CA	5.64	135.81	121.70
2	X	363	VAL	C-N-CA	5.64	135.81	121.70
2	X	187	PHE	CB-CG-CD1	5.62	124.73	120.80
1	P	409	ASP	CB-CG-OD1	5.59	123.33	118.30
2	X	365	SER	C-N-CA	5.58	135.66	121.70
1	P	379	PHE	CA-C-N	-5.57	104.94	117.20
1	P	258	ASP	CB-CG-OD1	-5.56	113.29	118.30
2	X	16	LYS	N-CA-CB	-5.55	100.60	110.60
1	P	319	ARG	CG-CD-NE	-5.55	100.15	111.80
1	P	544	ALA	C-N-CA	5.55	135.57	121.70
2	X	292	SER	CA-C-N	5.53	129.36	117.20
1	P	348	LYS	CG-CD-CE	5.52	128.47	111.90
2	X	169	PHE	CB-CG-CD1	5.52	124.67	120.80
2	X	227	ALA	C-N-CA	5.52	135.50	121.70
1	P	256	GLY	CA-C-N	5.51	129.32	117.20
1	P	480	HIS	C-N-CA	5.50	135.46	121.70
2	X	159	SER	N-CA-CB	-5.49	102.27	110.50
1	P	316	LYS	N-CA-CB	5.48	120.46	110.60
2	X	363	VAL	CG1-CB-CG2	5.47	119.66	110.90
1	P	307	TYR	CB-CG-CD1	5.46	124.27	121.00
2	X	161	ASN	O-C-N	-5.46	113.97	122.70
2	X	45	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	P	311	VAL	CB-CA-C	5.42	121.70	111.40
1	P	256	GLY	N-CA-C	5.38	126.56	113.10
2	X	41	LEU	CB-CA-C	5.37	120.40	110.20
2	X	200	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	P	309	SER	N-CA-CB	-5.37	102.45	110.50
1	P	626	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	X	273	ALA	N-CA-CB	5.36	117.60	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	62	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	X	162	THR	O-C-N	-5.34	114.16	122.70
2	X	166	LEU	O-C-N	-5.33	114.17	122.70
2	X	195	ARG	NE-CZ-NH2	-5.33	117.63	120.30
2	X	167	HIS	N-CA-CB	5.33	120.19	110.60
2	X	279	GLN	CA-CB-CG	5.32	125.10	113.40
1	P	449	TYR	CG-CD1-CE1	-5.30	117.06	121.30
1	P	684	GLU	CA-C-O	-5.29	108.98	120.10
2	X	421	SER	CA-C-O	-5.28	109.00	120.10
1	P	322	GLY	C-N-CA	5.27	134.88	121.70
2	X	368	PRO	C-N-CA	5.27	134.87	121.70
2	X	43	PRO	CA-N-CD	-5.25	104.15	111.50
1	P	286	VAL	CG1-CB-CG2	-5.22	102.55	110.90
2	X	21	LEU	CB-CA-C	-5.22	100.28	110.20
2	X	310	ASP	CB-CG-OD2	5.21	122.98	118.30
2	X	9	ILE	CB-CA-C	-5.20	101.20	111.60
1	P	542	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	X	17	LEU	CB-CA-C	5.18	120.05	110.20
1	P	550	VAL	CG1-CB-CG2	-5.17	102.64	110.90
2	X	278	VAL	CA-CB-CG2	5.15	118.63	110.90
2	X	339	ILE	CG1-CB-CG2	5.15	122.73	111.40
1	P	509	GLU	CB-CA-C	-5.15	100.11	110.40
1	P	596	ALA	C-N-CA	5.14	133.10	122.30
2	X	163	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	P	255	GLY	CA-C-N	5.13	126.47	116.20
2	X	157	SER	N-CA-CB	5.13	118.20	110.50
2	X	404	ILE	O-C-N	-5.13	114.47	123.20
2	X	302	ILE	N-CA-C	5.13	124.85	111.00
1	P	668	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	X	200	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	X	298	PHE	N-CA-CB	5.08	119.74	110.60
2	X	232	ASP	O-C-N	-5.07	114.59	122.70
2	X	326	ILE	CA-CB-CG2	-5.05	100.79	110.90
1	P	347	HIS	CA-CB-CG	5.05	122.19	113.60
2	X	163	ARG	CB-CA-C	5.04	120.48	110.40
2	X	27	ASN	C-N-CA	5.04	132.87	122.30
1	P	386	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	X	405	GLY	CA-C-N	5.01	128.22	117.20
1	P	548	GLU	OE1-CD-OE2	-5.00	117.30	123.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	142	LYS	CA

All (120) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	255	GLY	Mainchain
1	P	256	GLY	Peptide
1	P	257	LYS	Mainchain
1	P	260	VAL	Peptide
1	P	264	PHE	Mainchain
1	P	267	HIS	Mainchain
1	P	269	ASP	Sidechain
1	P	284	GLY	Mainchain
1	P	292	GLU	Sidechain
1	P	294	TYR	Sidechain
1	P	297	GLU	Sidechain,Mainchain
1	P	298	ALA	Peptide
1	P	299	LYS	Peptide
1	P	300	ASP	Peptide
1	P	301	ALA	Peptide
1	P	307	TYR	Sidechain
1	P	309	SER	Mainchain
1	P	311	VAL	Peptide
1	P	313	ASP	Mainchain
1	P	319	ARG	Sidechain,Peptide
1	P	321	ASP	Peptide
1	P	339	TYR	Sidechain,Peptide
1	P	340	THR	Mainchain,Peptide
1	P	345	PRO	Peptide
1	P	350	TYR	Sidechain
1	P	352	SER	Mainchain
1	P	353	GLU	Sidechain
1	P	354	MET	Peptide
1	P	358	ALA	Mainchain,Peptide
1	P	359	SER	Mainchain
1	P	360	GLN	Sidechain
1	P	362	ASP	Sidechain,Mainchain
1	P	364	GLY	Mainchain,Peptide
1	P	374	GLU	Sidechain
1	P	376	GLU	Mainchain
1	P	385	THR	Mainchain,Peptide
1	P	390	LEU	Peptide
1	P	391	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	P	392	ALA	Mainchain
1	P	400	MET	Peptide
1	P	408	ASP	Sidechain
1	P	410	PRO	Mainchain
1	P	429	PHE	Sidechain
1	P	439	THR	Mainchain
1	P	440	ASP	Peptide
1	P	446	VAL	Mainchain,Peptide
1	P	447	SER	Peptide
1	P	449	TYR	Sidechain
1	P	459	ASP	Peptide
1	P	460	PRO	Mainchain
1	P	472	LEU	Mainchain
1	P	473	GLU	Sidechain
1	P	476	ASP	Mainchain
1	P	482	ASP	Sidechain
1	P	484	HIS	Mainchain
1	P	505	GLU	Sidechain
1	P	509	GLU	Sidechain
1	P	511	GLY	Mainchain
1	P	512	HIS	Mainchain
1	P	534	TYR	Sidechain
1	P	536	GLU	Sidechain
1	P	538	GLU	Sidechain
1	P	539	ASN	Mainchain
1	P	542	ASP	Sidechain
1	P	543	MET	Mainchain
1	P	547	GLY	Peptide
1	P	548	GLU	Sidechain,Peptide
1	P	550	VAL	Peptide
1	P	561	ASP	Sidechain
1	P	576	LYS	Mainchain
1	P	589	GLU	Sidechain
1	P	590	LEU	Mainchain
1	P	600	CYS	Mainchain
1	P	621	GLU	Sidechain
1	P	625	ASN	Sidechain
1	P	630	LYS	Mainchain,Peptide
1	P	631	PRO	Mainchain
1	P	632	PRO	Peptide
1	P	646	GLU	Sidechain
1	P	657	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	P	659	TYR	Sidechain
1	P	664	ARG	Sidechain
1	P	668	ARG	Sidechain
1	P	669	ASP	Mainchain
2	X	114	TYR	Sidechain
2	X	141	ASP	Peptide
2	X	145	PHE	Sidechain
2	X	171	VAL	Peptide
2	X	173	LEU	Mainchain
2	X	177	HIS	Sidechain
2	X	189	ARG	Sidechain
2	X	198	TYR	Sidechain
2	X	226	SER	Mainchain
2	X	24	ALA	Mainchain
2	X	256	GLY	Peptide
2	X	269	ALA	Mainchain
2	X	274	ASN	Peptide
2	X	292	SER	Peptide
2	X	296	GLY	Peptide
2	X	298	PHE	Peptide
2	X	299	CYS	Mainchain
2	X	328	TYR	Sidechain
2	X	330	PHE	Sidechain
2	X	365	SER	Mainchain
2	X	367	GLU	Mainchain
2	X	404	ILE	Mainchain
2	X	45	TYR	Sidechain
2	X	61	SER	Peptide
2	X	65	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	P	3351	0	3391	331	0
2	X	3310	0	3337	425	0
3	P	32	0	12	56	0
All	All	6693	0	6740	740	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 55.

All (740) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:331:TYR:CZ	1:P:536:GLU:HG3	1.34	1.59
1:P:304:GLN:NE2	3:P:1685:GNP:H3'	1.15	1.47
2:X:352:ALA:CB	2:X:361:MET:HG3	1.46	1.44
2:X:343:GLU:HB3	2:X:344:PRO:CD	1.45	1.43
2:X:161:ASN:ND2	2:X:390:LYS:HB2	1.18	1.41
2:X:182:GLN:C	2:X:183:SER:N	1.71	1.41
2:X:354:ASP:HB3	2:X:357:THR:CG2	1.50	1.39
1:P:331:TYR:OH	1:P:536:GLU:C	1.63	1.37
1:P:271:GLY:HA3	3:P:1685:GNP:C8	1.51	1.36
1:P:271:GLY:CA	3:P:1685:GNP:H8	1.58	1.32
2:X:354:ASP:HB2	2:X:359:GLN:CD	1.48	1.30
2:X:183:SER:C	2:X:184:ALA:N	1.86	1.30
2:X:12:TRP:CZ3	2:X:321:GLU:OE2	1.88	1.25
1:P:331:TYR:CZ	1:P:536:GLU:CG	2.17	1.25
1:P:610:GLU:HG2	2:X:259:ASN:OD1	1.14	1.23
2:X:354:ASP:CB	2:X:357:THR:HG22	1.67	1.22
1:P:268:VAL:O	3:P:1685:GNP:O3A	1.53	1.22
1:P:331:TYR:OH	1:P:536:GLU:O	1.54	1.22
1:P:327:VAL:O	1:P:329:LYS:N	1.71	1.22
2:X:287:TYR:HE1	2:X:316:LYS:CB	1.52	1.21
2:X:161:ASN:HD22	2:X:390:LYS:CB	1.53	1.20
1:P:331:TYR:CE1	1:P:536:GLU:HG3	1.76	1.19
2:X:352:ALA:HB3	2:X:361:MET:CG	1.71	1.19
1:P:304:GLN:O	3:P:1685:GNP:O3'	1.59	1.19
2:X:354:ASP:N	2:X:359:GLN:HG2	1.56	1.19
2:X:287:TYR:CZ	2:X:316:LYS:HD3	1.77	1.18
2:X:287:TYR:HE1	2:X:316:LYS:HB3	1.03	1.18
1:P:304:GLN:CD	3:P:1685:GNP:H3'	1.60	1.18
2:X:287:TYR:OH	2:X:316:LYS:HD3	1.42	1.17
1:P:271:GLY:HA3	3:P:1685:GNP:N7	1.59	1.17
2:X:343:GLU:CB	2:X:344:PRO:HD2	1.73	1.17
2:X:106:LYS:N	2:X:106:LYS:HD2	1.45	1.16
1:P:271:GLY:CA	3:P:1685:GNP:C8	2.19	1.15
2:X:352:ALA:HB3	2:X:361:MET:HG3	1.16	1.15
2:X:354:ASP:H	2:X:359:GLN:CG	1.57	1.15
2:X:161:ASN:ND2	2:X:390:LYS:CB	2.08	1.14
2:X:163:ARG:HH22	2:X:391:SER:HA	1.02	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:304:GLN:NE2	3:P:1685:GNP:C3'	2.11	1.12
1:P:268:VAL:HG13	3:P:1685:GNP:O1B	1.49	1.11
1:P:307:TYR:CD2	3:P:1685:GNP:C2	2.20	1.11
2:X:354:ASP:HB2	2:X:359:GLN:NE2	1.65	1.10
2:X:183:SER:CA	2:X:184:ALA:N	2.13	1.10
2:X:308:ALA:HA	2:X:311:LEU:HD23	1.25	1.10
2:X:387:ILE:HG22	2:X:388:THR:H	1.06	1.09
2:X:104:GLU:O	2:X:105:LYS:HB3	1.50	1.09
2:X:326:ILE:HG22	2:X:327:ARG:H	1.05	1.09
1:P:328:GLY:HA2	1:P:350:TYR:CD2	1.88	1.08
2:X:308:ALA:HA	2:X:311:LEU:CD2	1.84	1.08
1:P:268:VAL:O	3:P:1685:GNP:PB	2.10	1.08
2:X:352:ALA:CB	2:X:361:MET:CG	2.30	1.08
1:P:328:GLY:HA2	1:P:350:TYR:CE2	1.88	1.07
2:X:343:GLU:HB3	2:X:344:PRO:HD2	1.08	1.07
2:X:267:LEU:HD13	2:X:267:LEU:H	0.93	1.06
2:X:353:ILE:CG1	2:X:361:MET:H	1.68	1.06
2:X:302:ILE:HB	2:X:401:PHE:HB3	1.36	1.06
2:X:287:TYR:CE1	2:X:316:LYS:CB	2.38	1.05
2:X:353:ILE:HG12	2:X:361:MET:N	1.70	1.05
2:X:183:SER:HB2	2:X:184:ALA:N	1.71	1.05
1:P:271:GLY:HA2	3:P:1685:GNP:H8	1.35	1.04
2:X:352:ALA:CA	2:X:361:MET:HG3	1.88	1.04
2:X:287:TYR:CE1	2:X:316:LYS:HB3	1.92	1.04
1:P:610:GLU:CG	2:X:259:ASN:OD1	2.04	1.03
2:X:105:LYS:O	2:X:105:LYS:HG2	1.58	1.03
2:X:387:ILE:CG2	2:X:388:THR:H	1.71	1.03
2:X:354:ASP:CB	2:X:357:THR:CG2	2.30	1.03
2:X:387:ILE:HG22	2:X:388:THR:N	1.70	1.02
2:X:100:GLU:HG3	2:X:101:ASP:N	1.72	1.01
2:X:343:GLU:HB3	2:X:344:PRO:HD3	1.44	1.00
1:P:268:VAL:CG1	3:P:1685:GNP:O1B	2.08	1.00
2:X:267:LEU:CD1	2:X:267:LEU:H	1.74	1.00
2:X:353:ILE:HG12	2:X:361:MET:H	0.85	0.99
2:X:267:LEU:HD13	2:X:267:LEU:N	1.72	0.99
2:X:352:ALA:C	2:X:361:MET:HG3	1.83	0.99
2:X:359:GLN:HG2	2:X:359:GLN:O	1.63	0.99
2:X:300:PHE:HD2	2:X:401:PHE:CZ	1.79	0.99
1:P:268:VAL:HG13	1:P:346:GLY:HA2	1.45	0.98
2:X:326:ILE:HG22	2:X:327:ARG:N	1.72	0.98
2:X:181:GLY:O	2:X:182:GLN:HG2	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:304:GLN:CD	3:P:1685:GNP:C3'	2.32	0.98
2:X:183:SER:CB	2:X:184:ALA:N	2.26	0.98
2:X:302:ILE:O	2:X:302:ILE:HG23	1.65	0.97
2:X:300:PHE:CD2	2:X:401:PHE:CE1	2.53	0.97
2:X:352:ALA:HB3	2:X:361:MET:CE	1.95	0.96
1:P:280:LEU:HD12	1:P:330:ALA:CB	1.96	0.95
2:X:350:SER:HA	2:X:361:MET:O	1.64	0.95
1:P:272:LYS:HG2	3:P:1685:GNP:O2B	1.65	0.94
1:P:597:GLY:HA3	2:X:396:GLN:HG2	1.49	0.94
2:X:326:ILE:HG21	2:X:367:GLU:O	1.67	0.94
2:X:352:ALA:HB3	2:X:361:MET:HE3	1.49	0.94
2:X:163:ARG:NH2	2:X:391:SER:HA	1.81	0.94
2:X:183:SER:C	2:X:184:ALA:CA	2.36	0.94
2:X:352:ALA:CB	2:X:361:MET:CE	2.46	0.94
2:X:409:ARG:HG2	2:X:409:ARG:HH11	1.33	0.94
2:X:354:ASP:CB	2:X:359:GLN:CD	2.36	0.94
2:X:106:LYS:N	2:X:106:LYS:CD	2.30	0.93
2:X:353:ILE:HG13	2:X:361:MET:HB2	1.51	0.92
2:X:12:TRP:CE3	2:X:321:GLU:OE2	2.20	0.92
1:P:331:TYR:OH	1:P:536:GLU:HG3	1.68	0.92
1:P:356:GLY:HA2	1:P:605:HIS:CE1	2.05	0.91
2:X:354:ASP:H	2:X:359:GLN:HG2	0.75	0.90
2:X:182:GLN:HG3	2:X:183:SER:N	1.86	0.89
2:X:287:TYR:CZ	2:X:316:LYS:CD	2.55	0.89
1:P:307:TYR:HD2	3:P:1685:GNP:C2	1.74	0.88
2:X:302:ILE:CB	2:X:401:PHE:HB3	2.03	0.88
2:X:343:GLU:N	2:X:346:ALA:HB3	1.88	0.88
1:P:348:LYS:NZ	3:P:1685:GNP:PG	2.46	0.88
1:P:330:ALA:C	1:P:341:ILE:HG22	1.94	0.87
1:P:330:ALA:HB3	1:P:341:ILE:HG21	1.54	0.87
1:P:280:LEU:HD12	1:P:330:ALA:HB2	1.57	0.86
1:P:328:GLY:HA2	1:P:350:TYR:CZ	2.10	0.86
1:P:304:GLN:HE22	3:P:1685:GNP:H3'	1.33	0.86
2:X:353:ILE:HA	2:X:359:GLN:O	1.75	0.85
2:X:301:GLY:HA3	2:X:401:PHE:CD2	2.11	0.85
2:X:182:GLN:CB	2:X:183:SER:N	2.39	0.85
2:X:300:PHE:CD2	2:X:401:PHE:CZ	2.64	0.84
2:X:342:ALA:HA	2:X:346:ALA:HB3	1.57	0.84
2:X:161:ASN:HB3	2:X:390:LYS:HD2	1.58	0.84
2:X:352:ALA:C	2:X:361:MET:CG	2.45	0.84
1:P:304:GLN:C	3:P:1685:GNP:HO3'	1.81	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:300:PHE:HD2	2:X:401:PHE:CE1	1.94	0.84
2:X:182:GLN:C	2:X:183:SER:CA	2.46	0.83
1:P:331:TYR:CE1	1:P:536:GLU:CG	2.54	0.83
1:P:528:VAL:HG21	1:P:554:ILE:HG23	1.57	0.83
2:X:287:TYR:CE1	2:X:316:LYS:HB2	2.13	0.83
2:X:354:ASP:HB3	2:X:357:THR:HG22	0.85	0.82
2:X:308:ALA:CA	2:X:311:LEU:HD23	2.09	0.82
1:P:328:GLY:O	1:P:329:LYS:HE3	1.79	0.82
2:X:352:ALA:O	2:X:359:GLN:HG3	1.78	0.81
1:P:330:ALA:HB3	1:P:341:ILE:CG2	2.09	0.81
2:X:263:GLN:OE1	2:X:267:LEU:HD21	1.79	0.81
2:X:106:LYS:HZ2	2:X:106:LYS:H	1.26	0.81
2:X:342:ALA:HA	2:X:346:ALA:CB	2.10	0.81
1:P:326:GLU:OE1	1:P:329:LYS:O	1.98	0.80
1:P:331:TYR:CE1	1:P:536:GLU:OE2	2.34	0.80
1:P:327:VAL:O	1:P:329:LYS:HB2	1.81	0.80
2:X:302:ILE:O	2:X:302:ILE:CG2	2.30	0.80
2:X:327:ARG:NH1	2:X:372:TRP:CD1	2.49	0.80
1:P:367:VAL:HG12	1:P:403:VAL:HG22	1.63	0.80
2:X:263:GLN:O	2:X:267:LEU:CD1	2.30	0.80
2:X:343:GLU:CB	2:X:344:PRO:CD	2.30	0.80
2:X:326:ILE:HG21	2:X:367:GLU:C	2.01	0.79
2:X:181:GLY:O	2:X:182:GLN:CG	2.30	0.79
2:X:311:LEU:O	2:X:311:LEU:HG	1.84	0.78
2:X:105:LYS:CG	2:X:105:LYS:O	2.30	0.78
2:X:352:ALA:O	2:X:359:GLN:CG	2.30	0.78
2:X:352:ALA:HB1	2:X:361:MET:HG3	1.64	0.78
1:P:361:ALA:HB3	1:P:397:VAL:HG23	1.66	0.78
2:X:287:TYR:CE1	2:X:316:LYS:CD	2.66	0.78
2:X:300:PHE:O	2:X:401:PHE:CE2	2.37	0.77
1:P:491:LEU:HD12	1:P:513:ILE:HD11	1.66	0.77
2:X:318:ILE:CG2	2:X:387:ILE:HD12	2.15	0.77
2:X:263:GLN:O	2:X:267:LEU:CD2	2.32	0.77
2:X:326:ILE:HD13	2:X:367:GLU:O	1.85	0.77
2:X:182:GLN:CG	2:X:183:SER:N	2.48	0.77
1:P:327:VAL:C	1:P:329:LYS:N	2.37	0.77
1:P:610:GLU:N	2:X:259:ASN:OD1	2.18	0.76
2:X:263:GLN:HG2	2:X:267:LEU:HD11	1.67	0.76
2:X:312:GLY:O	2:X:313:ALA:HB2	1.86	0.76
2:X:359:GLN:O	2:X:359:GLN:CG	2.32	0.76
1:P:405:ASN:OD1	3:P:1685:GNP:O6	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:610:GLU:HG2	2:X:259:ASN:CG	2.06	0.76
1:P:316:LYS:HG3	1:P:325:ILE:HG12	1.66	0.76
2:X:9:ILE:HG21	2:X:374:ALA:CB	2.16	0.76
2:X:354:ASP:N	2:X:359:GLN:CG	2.30	0.76
2:X:384:LEU:HD11	2:X:386:PHE:CE1	2.21	0.76
1:P:346:GLY:HA2	3:P:1685:GNP:O1B	1.87	0.75
2:X:270:GLU:O	2:X:271:ALA:HB3	1.86	0.75
2:X:315:GLU:HB2	2:X:409:ARG:HA	1.67	0.75
1:P:348:LYS:HZ2	3:P:1685:GNP:PG	2.10	0.75
1:P:273:SER:OG	1:P:325:ILE:HD12	1.86	0.75
2:X:182:GLN:CA	2:X:183:SER:N	2.50	0.75
1:P:587:ILE:HG22	1:P:675:ALA:HB2	1.67	0.74
2:X:343:GLU:O	2:X:347:LYS:HG3	1.87	0.74
2:X:354:ASP:CB	2:X:357:THR:HG21	2.17	0.74
2:X:409:ARG:HH11	2:X:409:ARG:CG	2.00	0.74
2:X:326:ILE:HG23	2:X:369:LEU:N	2.02	0.73
1:P:328:GLY:O	1:P:329:LYS:CE	2.35	0.73
2:X:104:GLU:O	2:X:105:LYS:CB	2.31	0.73
1:P:268:VAL:HG13	1:P:346:GLY:CA	2.17	0.73
1:P:550:VAL:HG23	1:P:552:LEU:HD11	1.69	0.73
1:P:277:GLY:HA2	1:P:326:GLU:OE2	1.89	0.73
1:P:605:HIS:CE1	1:P:661:GLN:NE2	2.56	0.73
1:P:348:LYS:NZ	3:P:1685:GNP:O2G	2.22	0.72
2:X:100:GLU:HG3	2:X:101:ASP:H	1.50	0.72
2:X:163:ARG:HH22	2:X:391:SER:CA	1.93	0.72
2:X:2:ASP:OD2	2:X:276:LYS:HG2	1.88	0.72
2:X:287:TYR:HB3	2:X:318:ILE:HD11	1.70	0.72
1:P:280:LEU:HG	1:P:331:TYR:H	1.51	0.72
1:P:326:GLU:HB2	1:P:343:ASP:OD2	1.90	0.72
1:P:331:TYR:CE2	1:P:536:GLU:CG	2.73	0.72
2:X:375:ALA:O	2:X:376:ASN:ND2	2.23	0.71
2:X:263:GLN:O	2:X:267:LEU:HD13	1.89	0.71
2:X:354:ASP:HB2	2:X:359:GLN:CG	2.20	0.71
2:X:105:LYS:C	2:X:106:LYS:HD2	2.09	0.71
2:X:352:ALA:HB3	2:X:361:MET:SD	2.30	0.71
2:X:327:ARG:NH1	2:X:372:TRP:NE1	2.39	0.70
2:X:379:ASN:ND2	2:X:379:ASN:OD1	2.24	0.70
1:P:319:ARG:HH12	1:P:324:THR:HG22	1.54	0.70
1:P:484:HIS:CE1	1:P:545:MET:HA	2.27	0.70
1:P:257:LYS:CD	1:P:258:ASP:H	2.04	0.70
2:X:263:GLN:O	2:X:267:LEU:HD22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:312:GLY:O	2:X:313:ALA:CB	2.40	0.70
2:X:287:TYR:CE1	2:X:316:LYS:HD3	2.25	0.70
2:X:302:ILE:HG12	2:X:401:PHE:CA	2.22	0.70
2:X:106:LYS:HD2	2:X:106:LYS:H	1.52	0.70
1:P:260:VAL:HG12	1:P:339:TYR:HA	1.74	0.69
1:P:327:VAL:O	1:P:328:GLY:C	2.30	0.69
1:P:307:TYR:CD2	3:P:1685:GNP:N1	2.59	0.69
1:P:328:GLY:CA	1:P:350:TYR:CZ	2.75	0.69
2:X:105:LYS:HA	2:X:106:LYS:NZ	2.07	0.69
2:X:145:PHE:CE2	2:X:265:ILE:HG12	2.28	0.69
1:P:299:LYS:HD3	1:P:311:VAL:H	1.57	0.69
1:P:330:ALA:O	1:P:341:ILE:HG22	1.91	0.69
1:P:328:GLY:C	1:P:350:TYR:CZ	2.66	0.69
2:X:181:GLY:C	2:X:182:GLN:HG2	2.13	0.69
2:X:389:ASP:HA	2:X:394:GLY:HA3	1.74	0.69
1:P:331:TYR:CE2	1:P:536:GLU:HG2	2.27	0.69
1:P:319:ARG:HH12	1:P:324:THR:CG2	2.06	0.68
1:P:308:LEU:HA	1:P:310:TRP:CE2	2.28	0.68
1:P:327:VAL:C	1:P:329:LYS:H	1.96	0.68
2:X:352:ALA:CB	2:X:361:MET:HE3	2.16	0.68
1:P:268:VAL:O	3:P:1685:GNP:O1B	2.12	0.68
2:X:354:ASP:CG	2:X:357:THR:CG2	2.62	0.68
2:X:330:PHE:CE1	2:X:364:VAL:HG22	2.28	0.67
2:X:339:ILE:HD12	2:X:349:LYS:HE3	1.76	0.67
2:X:354:ASP:N	2:X:359:GLN:CD	2.47	0.67
1:P:491:LEU:HD12	1:P:513:ILE:CD1	2.25	0.67
2:X:357:THR:HG23	2:X:359:GLN:H	1.58	0.67
1:P:392:ALA:HB1	1:P:397:VAL:HG11	1.76	0.67
1:P:605:HIS:CE1	1:P:661:GLN:HE22	2.12	0.67
1:P:304:GLN:CD	3:P:1685:GNP:O3'	2.33	0.66
2:X:333:ALA:C	2:X:335:ASP:H	1.99	0.66
2:X:270:GLU:O	2:X:271:ALA:CB	2.43	0.66
2:X:300:PHE:O	2:X:401:PHE:CZ	2.48	0.66
2:X:106:LYS:HZ2	2:X:106:LYS:N	1.93	0.66
2:X:328:TYR:CD2	2:X:364:VAL:HB	2.30	0.66
2:X:348:ASP:C	2:X:350:SER:H	1.98	0.66
1:P:273:SER:HB2	1:P:325:ILE:HB	1.77	0.66
2:X:288:PHE:HA	2:X:291:ILE:HD12	1.78	0.66
1:P:385:THR:HG21	1:P:429:PHE:CZ	2.31	0.66
2:X:302:ILE:HG12	2:X:401:PHE:HA	1.76	0.66
1:P:351:VAL:HG21	1:P:388:HIS:CB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:256:GLY:C	1:P:545:MET:HB3	2.15	0.65
2:X:267:LEU:N	2:X:267:LEU:CD1	2.44	0.65
2:X:354:ASP:N	2:X:359:GLN:OE1	2.30	0.65
1:P:356:GLY:CA	1:P:605:HIS:CE1	2.78	0.65
2:X:147:VAL:HG22	2:X:261:PHE:CE1	2.30	0.65
1:P:322:GLY:H	2:X:227:ALA:HB2	1.62	0.65
1:P:324:THR:HG23	1:P:348:LYS:HG2	1.78	0.65
1:P:597:GLY:HA2	1:P:614:VAL:HA	1.78	0.65
1:P:262:LEU:HD23	1:P:263:ILE:N	2.12	0.65
1:P:269:ASP:HA	3:P:1685:GNP:H5'2	1.79	0.65
1:P:331:TYR:OH	1:P:536:GLU:CA	2.46	0.64
2:X:333:ALA:O	2:X:335:ASP:N	2.30	0.64
1:P:331:TYR:CD1	1:P:536:GLU:OE2	2.50	0.64
2:X:104:GLU:OE1	2:X:105:LYS:N	2.30	0.64
1:P:521:LEU:HD11	1:P:566:PHE:HB3	1.80	0.64
2:X:342:ALA:C	2:X:346:ALA:HB3	2.18	0.64
2:X:4:GLU:CG	2:X:283:LEU:HD22	2.27	0.64
1:P:299:LYS:CD	1:P:311:VAL:H	2.11	0.64
2:X:101:ASP:O	2:X:103:LYS:N	2.30	0.64
2:X:390:LYS:O	2:X:391:SER:HB3	1.98	0.64
2:X:161:ASN:HD22	2:X:390:LYS:CG	2.09	0.64
2:X:326:ILE:HA	2:X:369:LEU:HB2	1.80	0.63
1:P:348:LYS:HE2	1:P:350:TYR:CD2	2.33	0.63
2:X:343:GLU:HB2	2:X:344:PRO:HD2	1.74	0.63
2:X:352:ALA:CB	2:X:361:MET:HE2	2.29	0.63
2:X:253:VAL:CG2	2:X:260:GLY:HA3	2.29	0.62
2:X:343:GLU:H	2:X:346:ALA:HB3	1.63	0.62
2:X:101:ASP:O	2:X:103:LYS:HD2	1.98	0.62
2:X:315:GLU:O	2:X:383:THR:OG1	2.03	0.62
2:X:387:ILE:CG2	2:X:388:THR:N	2.38	0.62
1:P:326:GLU:O	1:P:327:VAL:C	2.36	0.62
1:P:331:TYR:CZ	1:P:536:GLU:HG2	2.27	0.62
2:X:311:LEU:O	2:X:311:LEU:CG	2.48	0.62
1:P:288:LYS:HB2	1:P:291:ILE:HG22	1.82	0.61
2:X:352:ALA:O	2:X:359:GLN:CD	2.38	0.61
1:P:273:SER:CB	1:P:325:ILE:HB	2.30	0.61
2:X:323:LEU:HG	2:X:325:THR:H	1.64	0.61
2:X:298:PHE:CD2	2:X:300:PHE:HB3	2.36	0.61
2:X:319:VAL:O	2:X:386:PHE:HA	2.01	0.61
1:P:327:VAL:O	1:P:329:LYS:CB	2.48	0.61
2:X:352:ALA:CB	2:X:361:MET:SD	2.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:277:GLY:CA	1:P:326:GLU:OE2	2.48	0.61
1:P:322:GLY:H	2:X:227:ALA:CB	2.14	0.61
1:P:328:GLY:CA	1:P:350:TYR:CE2	2.75	0.60
1:P:521:LEU:HD22	1:P:562:ILE:HG13	1.82	0.60
2:X:100:GLU:CG	2:X:101:ASP:N	2.57	0.60
2:X:287:TYR:HE1	2:X:316:LYS:HB2	1.47	0.60
1:P:299:LYS:HD2	1:P:310:TRP:CE3	2.37	0.60
1:P:325:ILE:CD1	3:P:1685:GNP:O2A	2.50	0.60
1:P:615:LYS:HZ1	1:P:644:VAL:H	1.48	0.60
2:X:291:ILE:HG12	2:X:298:PHE:CD1	2.36	0.60
1:P:308:LEU:HB2	1:P:449:TYR:CE1	2.35	0.60
1:P:262:LEU:HD21	1:P:365:VAL:HG12	1.84	0.59
1:P:327:VAL:O	1:P:329:LYS:CA	2.49	0.59
2:X:105:LYS:HA	2:X:106:LYS:HZ3	1.67	0.59
1:P:272:LYS:N	3:P:1685:GNP:O1A	2.34	0.59
1:P:349:MET:HB3	2:X:255:TYR:HB2	1.84	0.59
2:X:264:ALA:HA	2:X:267:LEU:CD2	2.32	0.59
1:P:594:ILE:HG21	1:P:613:ILE:HG21	1.85	0.59
2:X:106:LYS:H	2:X:106:LYS:CD	2.11	0.59
2:X:163:ARG:HH12	2:X:391:SER:CB	2.15	0.59
2:X:182:GLN:HB2	2:X:183:SER:N	2.15	0.59
2:X:342:ALA:CA	2:X:346:ALA:HB3	2.32	0.59
2:X:348:ASP:O	2:X:350:SER:N	2.36	0.59
1:P:263:ILE:HG21	1:P:354:MET:SD	2.43	0.59
1:P:575:ILE:HG12	1:P:659:TYR:CE1	2.38	0.59
2:X:353:ILE:HG13	2:X:361:MET:CB	2.29	0.58
1:P:437:ILE:HG23	1:P:438:LYS:H	1.66	0.58
1:P:496:LYS:CE	1:P:502:THR:HG21	2.33	0.58
1:P:579:THR:HG22	1:P:580:LYS:H	1.68	0.58
2:X:302:ILE:HG12	2:X:401:PHE:CB	2.32	0.58
1:P:259:HIS:CD2	1:P:338:ARG:H	2.22	0.58
1:P:257:LYS:HE2	1:P:546:CYS:SG	2.43	0.58
2:X:223:LEU:HD11	2:X:233:LEU:HD12	1.86	0.58
2:X:299:CYS:C	2:X:406:ALA:H	2.06	0.58
2:X:354:ASP:O	2:X:357:THR:HG22	2.02	0.58
2:X:300:PHE:CE2	2:X:401:PHE:CE1	2.90	0.58
2:X:161:ASN:HD22	2:X:390:LYS:HB2	0.78	0.58
1:P:591:LYS:HA	1:P:591:LYS:HE3	1.86	0.58
2:X:12:TRP:CE3	2:X:321:GLU:CD	2.77	0.58
2:X:183:SER:C	2:X:184:ALA:HA	2.22	0.58
1:P:271:GLY:C	3:P:1685:GNP:O1A	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:615:LYS:HE3	1:P:644:VAL:HG23	1.86	0.57
2:X:389:ASP:HA	2:X:394:GLY:CA	2.33	0.57
2:X:174:PRO:HB3	2:X:194:LYS:HD2	1.86	0.57
2:X:104:GLU:CD	2:X:104:GLU:C	2.63	0.57
1:P:325:ILE:HD12	3:P:1685:GNP:O2A	2.04	0.57
1:P:355:ILE:HD12	1:P:392:ALA:H	1.68	0.57
1:P:554:ILE:CG2	1:P:557:VAL:HG12	2.35	0.57
2:X:161:ASN:O	2:X:390:LYS:HD3	2.05	0.57
2:X:263:GLN:OE1	2:X:267:LEU:CD2	2.52	0.57
2:X:330:PHE:CD1	2:X:364:VAL:HG13	2.40	0.57
1:P:344:ALA:O	3:P:1685:GNP:O2G	2.22	0.57
2:X:409:ARG:NH1	2:X:409:ARG:CG	2.63	0.57
2:X:314:VAL:CG1	2:X:406:ALA:HB1	2.35	0.56
1:P:550:VAL:CG2	1:P:552:LEU:HD11	2.34	0.56
2:X:106:LYS:H	2:X:106:LYS:NZ	2.00	0.56
1:P:487:ALA:HB1	1:P:488:PRO:HD2	1.87	0.56
2:X:300:PHE:O	2:X:401:PHE:CD2	2.58	0.56
1:P:299:LYS:HD2	1:P:310:TRP:HB2	1.87	0.56
1:P:389:ALA:HA	1:P:392:ALA:HB3	1.87	0.56
2:X:353:ILE:CG1	2:X:361:MET:N	2.49	0.56
2:X:416:GLN:HA	2:X:420:GLU:OE1	2.05	0.56
2:X:174:PRO:HG2	2:X:191:ARG:HA	1.88	0.56
2:X:326:ILE:CG2	2:X:327:ARG:N	2.56	0.56
2:X:333:ALA:C	2:X:335:ASP:N	2.59	0.56
2:X:174:PRO:N	2:X:194:LYS:HD3	2.21	0.55
2:X:389:ASP:CA	2:X:394:GLY:HA3	2.36	0.55
2:X:306:LEU:HD21	2:X:327:ARG:NE	2.21	0.55
2:X:319:VAL:HG21	2:X:373:LEU:HD13	1.86	0.55
1:P:271:GLY:HA2	3:P:1685:GNP:O5'	2.07	0.55
1:P:399:LYS:HG2	1:P:401:VAL:H	1.71	0.55
1:P:351:VAL:HG21	1:P:388:HIS:HB3	1.87	0.55
1:P:586:ALA:HB2	1:P:640:LYS:HD3	1.88	0.55
2:X:174:PRO:HD3	2:X:194:LYS:HB2	1.88	0.55
1:P:268:VAL:CA	3:P:1685:GNP:O1B	2.54	0.55
1:P:326:GLU:O	1:P:328:GLY:N	2.40	0.55
2:X:384:LEU:HD22	2:X:385:GLU:H	1.71	0.54
2:X:331:LYS:HG3	2:X:337:GLU:HB2	1.89	0.54
2:X:347:LYS:HA	2:X:363:VAL:HG11	1.88	0.54
1:P:356:GLY:HA2	1:P:605:HIS:NE2	2.20	0.54
2:X:330:PHE:CG	2:X:330:PHE:O	2.61	0.54
1:P:655:THR:HA	1:P:679:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:301:GLY:HA3	2:X:401:PHE:CG	2.42	0.53
2:X:161:ASN:HB3	2:X:390:LYS:CD	2.36	0.53
1:P:405:ASN:CG	3:P:1685:GNP:O6	2.47	0.53
1:P:597:GLY:HA3	2:X:396:GLN:CG	2.31	0.53
2:X:4:GLU:HG3	2:X:283:LEU:HD22	1.90	0.53
1:P:492:PRO:HD3	1:P:509:GLU:HG2	1.91	0.53
1:P:528:VAL:HG23	1:P:556:GLY:H	1.74	0.53
1:P:348:LYS:NZ	3:P:1685:GNP:O1G	2.35	0.53
1:P:405:ASN:ND2	3:P:1685:GNP:O6	2.41	0.53
2:X:161:ASN:ND2	2:X:390:LYS:CA	2.72	0.53
2:X:291:ILE:HG21	2:X:298:PHE:CD2	2.44	0.53
2:X:302:ILE:CG1	2:X:401:PHE:HB3	2.39	0.53
1:P:329:LYS:HA	1:P:329:LYS:HE3	1.90	0.52
1:P:255:GLY:N	1:P:545:MET:HG2	2.24	0.52
1:P:304:GLN:OE1	3:P:1685:GNP:O3'	2.27	0.52
1:P:323:LYS:HE3	2:X:253:VAL:O	2.09	0.52
2:X:171:VAL:HG11	2:X:198:TYR:CD1	2.44	0.52
2:X:317:LEU:HB3	2:X:384:LEU:HA	1.92	0.52
1:P:406:LYS:HA	3:P:1685:GNP:HN1	1.75	0.52
2:X:353:ILE:N	2:X:361:MET:HB2	2.24	0.52
1:P:259:HIS:CD2	1:P:338:ARG:N	2.78	0.52
1:P:304:GLN:HE22	3:P:1685:GNP:C5'	2.22	0.52
1:P:366:LEU:HD11	1:P:385:THR:HG23	1.90	0.52
1:P:365:VAL:HA	1:P:400:MET:O	2.09	0.52
1:P:582:VAL:HG12	1:P:644:VAL:HG22	1.91	0.52
1:P:616:LEU:HD13	1:P:624:THR:O	2.09	0.52
2:X:105:LYS:CA	2:X:106:LYS:HZ2	2.23	0.52
2:X:390:LYS:O	2:X:391:SER:CB	2.58	0.52
1:P:258:ASP:OD1	1:P:481:VAL:HG22	2.09	0.52
2:X:183:SER:HA	2:X:184:ALA:N	2.20	0.52
2:X:389:ASP:O	2:X:391:SER:N	2.43	0.52
1:P:626:ARG:HE	1:P:641:VAL:HG21	1.74	0.51
2:X:101:ASP:O	2:X:102:GLY:C	2.48	0.51
2:X:342:ALA:HA	2:X:346:ALA:HB1	1.89	0.51
1:P:356:GLY:HA3	1:P:605:HIS:CG	2.45	0.51
1:P:304:GLN:O	3:P:1685:GNP:C3'	2.56	0.51
1:P:324:THR:HG23	1:P:348:LYS:HE3	1.91	0.51
1:P:263:ILE:HG12	1:P:354:MET:HB3	1.93	0.51
1:P:575:ILE:CG1	1:P:659:TYR:CE1	2.94	0.51
2:X:30:SER:HB3	2:X:67:SER:HB3	1.93	0.51
2:X:9:ILE:CG2	2:X:374:ALA:CB	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:351:VAL:HG23	1:P:354:MET:HE3	1.91	0.51
2:X:174:PRO:CB	2:X:194:LYS:HD2	2.40	0.51
1:P:280:LEU:HB2	1:P:330:ALA:HB1	1.92	0.51
1:P:272:LYS:CG	3:P:1685:GNP:O2B	2.50	0.51
1:P:355:ILE:HD12	1:P:392:ALA:N	2.26	0.51
2:X:275:VAL:O	2:X:276:LYS:HG3	2.09	0.51
2:X:339:ILE:CD1	2:X:349:LYS:HE3	2.39	0.51
1:P:484:HIS:CE1	1:P:512:HIS:HA	2.46	0.51
1:P:268:VAL:HG12	3:P:1685:GNP:O1B	2.08	0.51
2:X:163:ARG:NH1	2:X:391:SER:HB3	2.26	0.51
2:X:308:ALA:O	2:X:311:LEU:O	2.29	0.51
1:P:586:ALA:HB1	1:P:631:PRO:CG	2.42	0.50
2:X:161:ASN:ND2	2:X:388:THR:OG1	2.44	0.50
1:P:269:ASP:O	3:P:1685:GNP:O4'	2.29	0.50
2:X:12:TRP:CD2	2:X:321:GLU:HB2	2.46	0.50
2:X:9:ILE:HD12	2:X:371:GLU:HA	1.94	0.50
1:P:304:GLN:OE1	3:P:1685:GNP:C3'	2.60	0.50
1:P:351:VAL:HG11	1:P:388:HIS:CE1	2.47	0.50
2:X:147:VAL:HG22	2:X:261:PHE:CZ	2.46	0.50
2:X:309:LEU:HD11	2:X:317:LEU:HD22	1.93	0.50
1:P:304:GLN:C	3:P:1685:GNP:O3'	2.41	0.50
1:P:324:THR:HG23	1:P:348:LYS:CG	2.40	0.50
2:X:105:LYS:O	2:X:106:LYS:O	2.30	0.50
2:X:251:VAL:HG11	2:X:264:ALA:HA	1.93	0.50
1:P:343:ASP:O	1:P:348:LYS:HE2	2.12	0.50
2:X:145:PHE:CE1	2:X:158:VAL:HG12	2.46	0.50
2:X:5:VAL:HG23	2:X:385:GLU:HB3	1.94	0.50
1:P:330:ALA:CA	1:P:341:ILE:HG22	2.41	0.50
1:P:324:THR:HG23	1:P:348:LYS:CD	2.42	0.50
2:X:103:LYS:O	2:X:104:GLU:OE2	2.30	0.50
2:X:354:ASP:HB3	2:X:357:THR:HG21	1.66	0.50
1:P:406:LYS:HE2	1:P:409:ASP:OD2	2.11	0.49
2:X:291:ILE:HG12	2:X:298:PHE:CG	2.47	0.49
2:X:352:ALA:O	2:X:359:GLN:OE1	2.30	0.49
2:X:354:ASP:CB	2:X:359:GLN:NE2	2.56	0.49
1:P:286:VAL:HG12	1:P:288:LYS:HE3	1.94	0.49
2:X:325:THR:HA	2:X:341:PHE:CB	2.42	0.49
2:X:353:ILE:HD11	2:X:362:ASP:OD1	2.13	0.49
2:X:354:ASP:CA	2:X:359:GLN:CD	2.80	0.49
2:X:35:VAL:HG22	2:X:91:VAL:HG13	1.94	0.49
1:P:319:ARG:NH1	1:P:327:VAL:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:316:LYS:CG	1:P:325:ILE:HG12	2.39	0.49
1:P:331:TYR:CE1	1:P:536:GLU:CD	2.86	0.49
1:P:437:ILE:HG23	1:P:438:LYS:N	2.28	0.49
2:X:347:LYS:O	2:X:363:VAL:HG21	2.12	0.49
2:X:354:ASP:CA	2:X:359:GLN:OE1	2.61	0.49
1:P:345:PRO:HA	1:P:348:LYS:HG3	1.94	0.49
2:X:291:ILE:O	2:X:291:ILE:HG22	2.13	0.49
2:X:4:GLU:HG2	2:X:283:LEU:HD22	1.94	0.49
1:P:255:GLY:O	1:P:545:MET:N	2.45	0.49
2:X:328:TYR:CE2	2:X:365:SER:O	2.65	0.49
1:P:268:VAL:HA	3:P:1685:GNP:O1B	2.13	0.49
1:P:259:HIS:CG	1:P:545:MET:CE	2.96	0.49
2:X:105:LYS:O	2:X:106:LYS:C	2.51	0.49
2:X:263:GLN:C	2:X:267:LEU:HD21	2.32	0.49
2:X:352:ALA:HB3	2:X:361:MET:CB	2.37	0.49
2:X:103:LYS:O	2:X:104:GLU:O	2.30	0.49
2:X:352:ALA:HB1	2:X:361:MET:CG	2.34	0.49
1:P:345:PRO:HA	1:P:348:LYS:CG	2.43	0.48
1:P:256:GLY:O	1:P:545:MET:HB3	2.14	0.48
2:X:72:ILE:HG22	2:X:76:GLN:HE21	1.78	0.48
2:X:105:LYS:CA	2:X:106:LYS:NZ	2.76	0.48
1:P:264:PHE:CE1	1:P:341:ILE:HD11	2.47	0.48
2:X:291:ILE:HD11	2:X:298:PHE:CE1	2.49	0.48
2:X:306:LEU:HD11	2:X:369:LEU:HD11	1.95	0.48
1:P:490:MET:HB2	1:P:509:GLU:HB2	1.96	0.48
1:P:575:ILE:HG12	1:P:659:TYR:CZ	2.49	0.48
2:X:326:ILE:HG12	2:X:368:PRO:HA	1.95	0.48
2:X:384:LEU:HD22	2:X:385:GLU:N	2.27	0.48
2:X:53:TYR:CE1	2:X:69:LEU:HG	2.49	0.48
1:P:409:ASP:HB3	3:P:1685:GNP:HN21	1.79	0.48
1:P:257:LYS:HD3	1:P:258:ASP:H	1.78	0.48
1:P:507:LYS:CE	1:P:547:GLY:HA2	2.43	0.48
2:X:314:VAL:HG11	2:X:406:ALA:HB1	1.96	0.48
2:X:287:TYR:CE1	2:X:316:LYS:HD2	2.46	0.48
2:X:311:LEU:O	2:X:312:GLY:C	2.52	0.48
2:X:338:VAL:O	2:X:339:ILE:HD13	2.14	0.48
2:X:9:ILE:HD12	2:X:370:ILE:HG22	1.96	0.48
1:P:257:LYS:HD2	1:P:258:ASP:H	1.77	0.48
1:P:605:HIS:CE1	1:P:661:GLN:CD	2.87	0.48
2:X:300:PHE:HA	2:X:405:GLY:HA3	1.96	0.48
1:P:271:GLY:N	3:P:1685:GNP:C8	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:330:ALA:CB	1:P:341:ILE:CG2	2.87	0.48
2:X:163:ARG:HH12	2:X:391:SER:HB2	1.77	0.48
1:P:316:LYS:O	1:P:316:LYS:HG2	2.14	0.48
1:P:619:LYS:HG2	1:P:620:LEU:HD12	1.96	0.48
2:X:348:ASP:C	2:X:350:SER:N	2.65	0.48
2:X:9:ILE:CD1	2:X:371:GLU:HA	2.44	0.47
2:X:383:THR:HG22	2:X:384:LEU:H	1.78	0.47
2:X:186:ARG:HG2	2:X:186:ARG:O	2.14	0.47
2:X:251:VAL:HG11	2:X:264:ALA:CB	2.45	0.47
2:X:253:VAL:CG2	2:X:260:GLY:CA	2.93	0.47
2:X:300:PHE:CE2	2:X:401:PHE:HE1	2.31	0.47
2:X:95:GLY:O	2:X:106:LYS:HB2	2.13	0.47
2:X:174:PRO:HD3	2:X:194:LYS:CB	2.44	0.47
2:X:325:THR:HA	2:X:341:PHE:HB2	1.96	0.47
1:P:324:THR:CG2	1:P:348:LYS:HE3	2.45	0.47
1:P:545:MET:HG3	1:P:546:CYS:O	2.14	0.47
1:P:257:LYS:HA	1:P:545:MET:SD	2.54	0.47
2:X:327:ARG:HG2	2:X:369:LEU:HG	1.96	0.47
1:P:385:THR:HG21	1:P:429:PHE:CE2	2.49	0.47
1:P:596:ALA:HB1	1:P:615:LYS:HA	1.97	0.47
1:P:391:LEU:HD23	1:P:603:HIS:HD1	1.79	0.47
2:X:142:LYS:HB2	2:X:159:SER:HA	1.97	0.47
2:X:384:LEU:HD22	2:X:385:GLU:O	2.14	0.47
1:P:259:HIS:HB3	1:P:338:ARG:HB2	1.97	0.47
1:P:406:LYS:NZ	3:P:1685:GNP:N3	2.56	0.47
2:X:263:GLN:CD	2:X:267:LEU:HD21	2.35	0.47
1:P:317:GLU:O	1:P:321:ASP:OD1	2.33	0.47
1:P:496:LYS:HE2	1:P:502:THR:HG21	1.96	0.47
2:X:298:PHE:CE2	2:X:300:PHE:HB3	2.50	0.47
2:X:407:MET:HE3	2:X:407:MET:HB3	1.74	0.47
1:P:280:LEU:HD12	1:P:330:ALA:CA	2.45	0.47
1:P:331:TYR:HB2	1:P:339:TYR:O	2.14	0.47
2:X:104:GLU:OE1	2:X:106:LYS:NZ	2.48	0.47
2:X:301:GLY:N	2:X:404:ILE:O	2.48	0.47
2:X:386:PHE:C	2:X:387:ILE:HG13	2.35	0.47
1:P:659:TYR:CD1	1:P:659:TYR:N	2.83	0.47
2:X:327:ARG:CZ	2:X:372:TRP:CD1	2.98	0.46
2:X:253:VAL:HG21	2:X:260:GLY:C	2.35	0.46
2:X:275:VAL:C	2:X:276:LYS:HG3	2.36	0.46
2:X:161:ASN:CG	2:X:390:LYS:HB2	2.17	0.46
1:P:255:GLY:O	1:P:544:ALA:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:293:GLN:C	2:X:295:THR:H	2.18	0.46
2:X:339:ILE:CG1	2:X:349:LYS:HE3	2.45	0.46
2:X:416:GLN:O	2:X:417:LEU:HD23	2.16	0.46
2:X:9:ILE:O	2:X:9:ILE:HG12	2.16	0.46
1:P:366:LEU:HA	1:P:366:LEU:HD13	1.73	0.46
2:X:358:GLY:O	2:X:360:GLU:N	2.47	0.46
1:P:348:LYS:HZ3	3:P:1685:GNP:PG	2.37	0.46
1:P:260:VAL:CG1	1:P:339:TYR:HA	2.45	0.46
1:P:342:LEU:HD12	1:P:358:ALA:HB3	1.98	0.46
1:P:605:HIS:CE1	1:P:661:GLN:OE1	2.69	0.46
2:X:345:GLU:O	2:X:349:LYS:N	2.49	0.46
1:P:577:SER:HB2	1:P:652:CYS:HA	1.97	0.46
2:X:354:ASP:CG	2:X:357:THR:HG22	2.27	0.46
1:P:603:HIS:HB2	1:P:666:THR:HG22	1.97	0.46
2:X:174:PRO:CG	2:X:194:LYS:HD2	2.46	0.46
2:X:331:LYS:HD3	2:X:337:GLU:HB2	1.98	0.46
1:P:271:GLY:CA	3:P:1685:GNP:O1A	2.63	0.46
1:P:366:LEU:HD22	1:P:400:MET:HG3	1.98	0.46
1:P:484:HIS:HE1	1:P:512:HIS:HA	1.81	0.46
1:P:255:GLY:CA	1:P:545:MET:HE2	2.46	0.46
2:X:330:PHE:CD1	2:X:330:PHE:O	2.69	0.46
2:X:302:ILE:HG12	2:X:401:PHE:HB3	1.96	0.46
1:P:325:ILE:HD11	3:P:1685:GNP:O2A	2.16	0.46
1:P:332:PHE:CE2	1:P:454:LEU:HD23	2.51	0.46
2:X:78:LYS:HG3	2:X:108:THR:HG23	1.98	0.46
2:X:287:TYR:HB3	2:X:318:ILE:CD1	2.43	0.46
1:P:319:ARG:HH22	1:P:324:THR:HG21	1.81	0.45
1:P:348:LYS:CD	1:P:350:TYR:HB2	2.45	0.45
1:P:620:LEU:HD12	1:P:620:LEU:H	1.82	0.45
1:P:256:GLY:O	1:P:484:HIS:CG	2.69	0.45
2:X:158:VAL:HG11	2:X:265:ILE:HG21	1.98	0.45
2:X:354:ASP:CB	2:X:359:GLN:CG	2.91	0.45
1:P:578:VAL:HG12	1:P:579:THR:N	2.31	0.45
2:X:147:VAL:CG2	2:X:261:PHE:CZ	2.99	0.45
2:X:7:LYS:HE3	2:X:277:TYR:CE1	2.51	0.45
2:X:331:LYS:CE	2:X:361:MET:SD	3.04	0.45
1:P:343:ASP:OD2	1:P:350:TYR:HE2	2.00	0.45
2:X:373:LEU:O	2:X:384:LEU:HG	2.16	0.45
1:P:502:THR:HG23	1:P:559:GLU:OE1	2.17	0.45
2:X:174:PRO:CG	2:X:191:ARG:HA	2.46	0.45
2:X:362:ASP:O	2:X:363:VAL:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:12:TRP:CE2	2:X:321:GLU:HB2	2.52	0.45
2:X:328:TYR:HB3	2:X:364:VAL:HG21	1.98	0.45
1:P:298:ALA:HB3	1:P:299:LYS:HZ3	1.81	0.45
1:P:323:LYS:CE	2:X:253:VAL:O	2.64	0.45
2:X:2:ASP:OD2	2:X:276:LYS:CG	2.62	0.45
2:X:331:LYS:HE3	2:X:361:MET:SD	2.57	0.45
1:P:355:ILE:HG23	1:P:356:GLY:H	1.82	0.45
1:P:371:ARG:HB2	1:P:410:PRO:CG	2.47	0.45
2:X:263:GLN:C	2:X:267:LEU:CD2	2.86	0.45
2:X:354:ASP:O	2:X:357:THR:N	2.49	0.45
2:X:299:CYS:O	2:X:406:ALA:N	2.50	0.45
2:X:38:PRO:HA	2:X:85:LEU:CD1	2.47	0.45
1:P:657:GLN:HG3	1:P:678:LYS:HZ1	1.82	0.45
2:X:125:ASP:CG	2:X:126:ASN:H	2.20	0.45
2:X:353:ILE:CG1	2:X:361:MET:HB2	2.36	0.45
1:P:256:GLY:N	1:P:545:MET:HE2	2.32	0.45
1:P:549:GLN:HG2	1:P:550:VAL:N	2.31	0.45
2:X:352:ALA:O	2:X:361:MET:CG	2.65	0.45
1:P:540:GLU:O	1:P:541:VAL:HG22	2.16	0.44
1:P:585:ILE:O	1:P:641:VAL:HG12	2.17	0.44
1:P:319:ARG:NH1	1:P:324:THR:CG2	2.76	0.44
2:X:317:LEU:HD21	2:X:373:LEU:HD13	1.99	0.44
2:X:301:GLY:HA2	2:X:404:ILE:H	1.83	0.44
1:P:328:GLY:HA2	1:P:350:TYR:CE1	2.53	0.44
1:P:352:SER:HB2	1:P:606:THR:O	2.18	0.44
2:X:158:VAL:HG11	2:X:265:ILE:CG2	2.48	0.44
2:X:286:ALA:O	2:X:290:GLU:HB2	2.16	0.44
2:X:352:ALA:C	2:X:361:MET:HG2	2.36	0.44
1:P:349:MET:HE2	2:X:255:TYR:O	2.17	0.44
2:X:354:ASP:CG	2:X:357:THR:HG21	2.33	0.44
1:P:333:GLU:HB2	1:P:338:ARG:CG	2.48	0.44
1:P:331:TYR:OH	1:P:536:GLU:CG	2.47	0.44
2:X:291:ILE:CD1	2:X:298:PHE:CE1	3.00	0.44
1:P:354:MET:CE	1:P:392:ALA:HB2	2.48	0.44
2:X:357:THR:CG2	2:X:359:GLN:H	2.28	0.44
2:X:9:ILE:HD11	2:X:371:GLU:HG2	2.00	0.44
1:P:283:THR:HG21	1:P:333:GLU:HB3	1.98	0.44
2:X:300:PHE:CG	2:X:300:PHE:O	2.70	0.43
2:X:343:GLU:H	2:X:346:ALA:CB	2.31	0.43
2:X:6:GLU:HG2	2:X:384:LEU:O	2.18	0.43
1:P:308:LEU:HA	1:P:310:TRP:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:463:CYS:SG	1:P:464:PRO:HD3	2.58	0.43
1:P:536:GLU:HB3	1:P:548:GLU:CD	2.37	0.43
2:X:319:VAL:O	2:X:386:PHE:CA	2.65	0.43
1:P:259:HIS:CG	1:P:338:ARG:H	2.35	0.43
1:P:259:HIS:HB2	1:P:545:MET:SD	2.59	0.43
2:X:280:GLU:CB	2:X:284:LEU:HG	2.48	0.43
1:P:298:ALA:C	1:P:299:LYS:HG3	2.38	0.43
1:P:351:VAL:HG21	1:P:388:HIS:CG	2.53	0.43
1:P:496:LYS:HZ3	1:P:502:THR:HG21	1.83	0.43
2:X:277:TYR:HB2	2:X:278:VAL:HG13	1.99	0.43
2:X:331:LYS:HE2	2:X:332:ASP:HB2	2.00	0.43
1:P:262:LEU:C	1:P:262:LEU:HD23	2.39	0.43
1:P:610:GLU:CA	2:X:259:ASN:OD1	2.66	0.43
2:X:9:ILE:CD1	2:X:370:ILE:HG22	2.49	0.43
1:P:259:HIS:CE1	1:P:545:MET:HE1	2.54	0.43
1:P:259:HIS:O	1:P:547:GLY:HA3	2.18	0.43
1:P:440:ASP:O	1:P:441:VAL:HG13	2.19	0.43
1:P:261:SER:HA	1:P:507:LYS:NZ	2.34	0.43
1:P:391:LEU:CD2	1:P:608:ILE:HD11	2.49	0.43
2:X:264:ALA:HA	2:X:267:LEU:HD22	2.01	0.43
2:X:6:GLU:HA	2:X:385:GLU:HA	1.99	0.43
1:P:342:LEU:HD21	1:P:350:TYR:O	2.18	0.43
1:P:510:SER:CA	1:P:546:CYS:HB2	2.48	0.43
1:P:510:SER:HA	1:P:546:CYS:HB2	2.01	0.43
1:P:307:TYR:O	1:P:449:TYR:HA	2.19	0.43
2:X:147:VAL:CG2	2:X:261:PHE:CE1	3.01	0.43
2:X:326:ILE:HG23	2:X:369:LEU:H	1.82	0.43
1:P:257:LYS:HE2	1:P:546:CYS:CB	2.49	0.43
1:P:460:PRO:O	1:P:461:LYS:HB2	2.19	0.43
1:P:460:PRO:CG	1:P:462:GLU:HG2	2.49	0.43
1:P:540:GLU:O	1:P:541:VAL:HG13	2.19	0.43
2:X:182:GLN:C	2:X:183:SER:HA	2.34	0.43
1:P:349:MET:HB3	2:X:255:TYR:CB	2.49	0.43
1:P:487:ALA:HB1	1:P:488:PRO:CD	2.48	0.43
2:X:163:ARG:NH1	2:X:391:SER:CB	2.81	0.43
1:P:351:VAL:HG22	1:P:391:LEU:CD1	2.49	0.42
1:P:399:LYS:HB2	1:P:440:ASP:HB2	2.01	0.42
2:X:132:VAL:HA	2:X:135:GLU:CB	2.50	0.42
2:X:287:TYR:CD1	2:X:318:ILE:HD11	2.54	0.42
2:X:287:TYR:O	2:X:291:ILE:CD1	2.67	0.42
2:X:314:VAL:HG12	2:X:406:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:43:PRO:HA	2:X:46:GLN:HB2	2.01	0.42
1:P:365:VAL:HA	1:P:400:MET:HB2	2.00	0.42
2:X:155:PHE:CZ	2:X:205:VAL:CG2	3.02	0.42
2:X:291:ILE:O	2:X:291:ILE:CG2	2.65	0.42
2:X:326:ILE:H	2:X:341:PHE:H	1.67	0.42
1:P:297:GLU:O	1:P:299:LYS:HE2	2.18	0.42
2:X:101:ASP:C	2:X:103:LYS:N	2.73	0.42
2:X:174:PRO:HG3	2:X:194:LYS:HD2	2.01	0.42
2:X:263:GLN:O	2:X:267:LEU:HD11	2.16	0.42
2:X:354:ASP:HB2	2:X:359:GLN:HB3	2.02	0.42
1:P:299:LYS:CD	1:P:310:TRP:HB2	2.49	0.42
1:P:342:LEU:C	1:P:342:LEU:HD23	2.40	0.42
1:P:458:VAL:C	1:P:460:PRO:HD3	2.39	0.42
1:P:491:LEU:HG	1:P:508:ILE:HG22	2.01	0.42
2:X:328:TYR:HB2	2:X:339:ILE:HB	2.00	0.42
2:X:147:VAL:CG2	2:X:154:LEU:HB3	2.49	0.42
2:X:298:PHE:CD1	2:X:299:CYS:O	2.73	0.42
1:P:299:LYS:HD3	1:P:311:VAL:N	2.29	0.42
1:P:328:GLY:C	1:P:350:TYR:OH	2.58	0.42
2:X:160:GLY:HA2	2:X:278:VAL:HB	2.01	0.42
2:X:9:ILE:HG21	2:X:374:ALA:HB3	2.00	0.42
1:P:308:LEU:HB2	1:P:449:TYR:CD1	2.54	0.42
2:X:123:LEU:HD12	2:X:129:HIS:H	1.85	0.42
2:X:280:GLU:HG2	2:X:284:LEU:HG	2.02	0.42
1:P:264:PHE:CE2	1:P:365:VAL:HG11	2.54	0.42
1:P:310:TRP:HB3	1:P:313:ASP:HB2	2.01	0.42
1:P:324:THR:HG23	1:P:348:LYS:CE	2.50	0.42
2:X:104:GLU:CD	2:X:105:LYS:N	2.73	0.42
2:X:288:PHE:HA	2:X:291:ILE:CD1	2.48	0.42
2:X:352:ALA:O	2:X:361:MET:HG2	2.20	0.42
1:P:594:ILE:CG1	1:P:674:ILE:HD13	2.50	0.41
2:X:30:SER:HB2	2:X:71:ALA:HB2	2.01	0.41
2:X:9:ILE:HB	2:X:386:PHE:CE1	2.55	0.41
1:P:351:VAL:HG21	1:P:388:HIS:CA	2.50	0.41
1:P:275:MET:SD	1:P:403:VAL:HG21	2.60	0.41
1:P:346:GLY:H	1:P:348:LYS:HG3	1.86	0.41
2:X:354:ASP:CB	2:X:359:GLN:HB3	2.50	0.41
1:P:264:PHE:HE1	1:P:341:ILE:HD11	1.85	0.41
1:P:345:PRO:HB2	1:P:384:GLN:OE1	2.20	0.41
1:P:268:VAL:HG22	1:P:347:HIS:H	1.85	0.41
1:P:263:ILE:HD12	1:P:361:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:507:LYS:HE2	1:P:547:GLY:HA2	2.01	0.41
2:X:155:PHE:CZ	2:X:205:VAL:HG23	2.56	0.41
1:P:610:GLU:CB	2:X:259:ASN:OD1	2.65	0.41
2:X:386:PHE:O	2:X:387:ILE:HG13	2.20	0.41
2:X:287:TYR:CB	2:X:318:ILE:HD11	2.44	0.41
2:X:284:LEU:CD2	2:X:387:ILE:HD11	2.50	0.41
1:P:304:GLN:OE1	3:P:1685:GNP:H5'1	2.21	0.41
1:P:277:GLY:N	1:P:326:GLU:OE2	2.54	0.41
1:P:345:PRO:HG2	1:P:388:HIS:CE1	2.56	0.41
1:P:345:PRO:HG2	1:P:388:HIS:ND1	2.36	0.41
1:P:484:HIS:ND1	1:P:544:ALA:O	2.54	0.41
1:P:609:GLU:HA	2:X:259:ASN:HD21	1.86	0.41
2:X:319:VAL:HG21	2:X:373:LEU:CD1	2.51	0.41
2:X:317:LEU:O	2:X:385:GLU:N	2.52	0.41
1:P:333:GLU:HA	1:P:338:ARG:HA	2.03	0.41
1:P:363:VAL:HG11	1:P:475:LEU:HD22	2.02	0.41
1:P:258:ASP:OD1	1:P:481:VAL:N	2.54	0.41
2:X:338:VAL:C	2:X:339:ILE:HD13	2.41	0.41
2:X:352:ALA:HB1	2:X:361:MET:SD	2.61	0.41
1:P:309:SER:HB2	1:P:448:GLY:C	2.41	0.41
1:P:586:ALA:HB1	1:P:631:PRO:HG3	2.02	0.41
1:P:663:GLY:HA2	1:P:679:ILE:HG22	2.03	0.41
2:X:248:ILE:CG2	2:X:249:SER:N	2.84	0.41
2:X:258:GLU:CD	2:X:258:GLU:H	2.24	0.41
2:X:263:GLN:O	2:X:267:LEU:HD21	2.19	0.41
2:X:326:ILE:HG23	2:X:368:PRO:C	2.41	0.41
1:P:312:MET:HA	1:P:312:MET:CE	2.51	0.41
2:X:211:ILE:HA	2:X:216:VAL:HA	2.02	0.41
2:X:283:LEU:O	2:X:287:TYR:CD2	2.73	0.41
1:P:356:GLY:CA	1:P:605:HIS:CD2	3.04	0.41
1:P:355:ILE:CD1	1:P:392:ALA:H	2.32	0.41
1:P:279:LEU:O	1:P:332:PHE:CD2	2.74	0.40
1:P:616:LEU:C	1:P:616:LEU:HD23	2.42	0.40
2:X:21:LEU:HD21	2:X:93:TYR:CD2	2.56	0.40
2:X:353:ILE:CA	2:X:359:GLN:O	2.58	0.40
2:X:392:SER:OG	2:X:393:GLU:OE2	2.30	0.40
1:P:586:ALA:HB1	1:P:631:PRO:HG2	2.04	0.40
2:X:145:PHE:CE2	2:X:222:ILE:HG12	2.56	0.40
2:X:306:LEU:HD21	2:X:327:ARG:HE	1.84	0.40
2:X:335:ASP:HB3	2:X:336:ASN:H	1.63	0.40
1:P:330:ALA:CB	1:P:341:ILE:HG22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:319:VAL:HB	2:X:386:PHE:CD2	2.56	0.40
1:P:283:THR:HG23	1:P:333:GLU:O	2.22	0.40
1:P:618:HIS:HB2	1:P:642:ILE:HG22	2.04	0.40
1:P:268:VAL:C	3:P:1685:GNP:O1B	2.59	0.40
1:P:257:LYS:HE2	1:P:546:CYS:HB3	2.03	0.40
2:X:286:ALA:HB1	2:X:290:GLU:OE2	2.22	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 PDB entries followed by that with respect to all EM entries.

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	P	428/430 (100%)	299 (70%)	69 (16%)	60 (14%)	0	6
2	X	420/437 (96%)	297 (71%)	58 (14%)	65 (16%)	0	5
All	All	848/867 (98%)	596 (70%)	127 (15%)	125 (15%)	1	6

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	258	ASP
1	P	260	VAL
1	P	285	SER
1	P	298	ALA
1	P	300	ASP
1	P	308	LEU
1	P	309	SER
1	P	310	TRP
1	P	312	MET
1	P	321	ASP
1	P	327	VAL
1	P	328	GLY

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Mol	Chain	Res	Type
1	P	345	PRO
1	P	397	VAL
1	P	411	THR
1	P	437	ILE
1	P	478	MET
1	P	485	ILE
1	P	535	ASN
1	P	541	VAL
1	P	572	LYS
1	P	579	THR
1	P	628	SER
2	X	25	ARG
2	X	26	GLY
2	X	104	GLU
2	X	105	LYS
2	X	139	ALA
2	X	142	LYS
2	X	166	LEU
2	X	167	HIS
2	X	185	LEU
2	X	186	ARG
2	X	240	ASP
2	X	257	GLY
2	X	268	SER
2	X	269	ALA
2	X	273	ALA
2	X	275	VAL
2	X	279	GLN
2	X	282	LYS
2	X	313	ALA
2	X	330	PHE
2	X	334	GLU
2	X	343	GLU
2	X	363	VAL
2	X	364	VAL
2	X	370	ILE
2	X	377	TYR
2	X	409	ARG
1	P	281	TYR
1	P	282	LEU
1	P	286	VAL
1	P	297	GLU

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Mol	Chain	Res	Type
1	P	364	GLY
1	P	383	GLY
1	P	392	ALA
1	P	399	LYS
1	P	401	VAL
1	P	441	VAL
1	P	453	ASN
1	P	461	LYS
1	P	481	VAL
1	P	483	ARG
1	P	486	ASN
1	P	525	LYS
1	P	621	GLU
2	X	5	VAL
2	X	28	GLY
2	X	98	ILE
2	X	99	THR
2	X	102	GLY
2	X	106	LYS
2	X	131	GLU
2	X	176	LYS
2	X	241	PRO
2	X	255	TYR
2	X	276	LYS
2	X	281	LYS
2	X	296	GLY
2	X	312	GLY
2	X	341	PHE
2	X	349	LYS
2	X	359	GLN
2	X	387	ILE
2	X	390	LYS
2	X	391	SER
1	P	287	ASP
1	P	318	GLU
1	P	372	LYS
1	P	400	MET
1	P	452	ALA
1	P	636	LYS
1	P	638	GLY
1	P	652	CYS
2	X	113	PRO

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Mol	Chain	Res	Type
2	X	138	GLN
2	X	213	ASN
2	X	220	GLY
2	X	221	LEU
2	X	270	GLU
2	X	274	ASN
2	X	294	ASP
2	X	295	THR
2	X	411	LYS
1	P	303	ARG
1	P	320	ASN
2	X	266	GLU
1	P	359	SER
1	P	571	PRO
1	P	630	LYS
1	P	631	PRO
2	X	120	SER
2	X	132	VAL
2	X	184	ALA
2	X	271	ALA
2	X	305	THR
2	X	365	SER
1	P	360	GLN
1	P	574	PRO
1	P	669	ASP
2	X	215	LYS
1	P	575	ILE
1	P	588	VAL
1	P	604	VAL

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 PDB entries followed by that with respect to all EM entries.

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	P	365/365 (100%)	304 (83%)	61 (17%)	3	19
2	X	362/377 (96%)	290 (80%)	72 (20%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	727/742 (98%)	594 (82%)	133 (18%)	5 14

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	257	LYS
1	P	260	VAL
1	P	272	LYS
1	P	286	VAL
1	P	288	LYS
1	P	289	ARG
1	P	296	ARG
1	P	306	TRP
1	P	307	TYR
1	P	310	TRP
1	P	312	MET
1	P	314	THR
1	P	320	ASN
1	P	329	LYS
1	P	332	PHE
1	P	340	THR
1	P	343	ASP
1	P	350	TYR
1	P	366	LEU
1	P	372	LYS
1	P	374	GLU
1	P	375	TYR
1	P	377	THR
1	P	381	ARG
1	P	384	GLN
1	P	386	ARG
1	P	394	THR
1	P	395	GLN
1	P	400	MET
1	P	409	ASP
1	P	410	PRO
1	P	412	VAL
1	P	417	GLU
1	P	428	ASN
1	P	437	ILE
1	P	440	ASP
1	P	442	VAL

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Mol	Chain	Res	Type
1	P	449	TYR
1	P	482	ASP
1	P	485	ILE
1	P	530	ILE
1	P	536	GLU
1	P	542	ASP
1	P	549	GLN
1	P	557	VAL
1	P	562	ILE
1	P	576	LYS
1	P	577	SER
1	P	580	LYS
1	P	589	GLU
1	P	590	LEU
1	P	591	LYS
1	P	605	HIS
1	P	615	LYS
1	P	637	LYS
1	P	642	ILE
1	P	652	CYS
1	P	655	THR
1	P	661	GLN
1	P	678	LYS
1	P	681	LYS
2	X	13	LYS
2	X	25	ARG
2	X	41	LEU
2	X	42	ILE
2	X	43	PRO
2	X	50	THR
2	X	58	ASN
2	X	65	ARG
2	X	79	LEU
2	X	87	LYS
2	X	90	LEU
2	X	92	LEU
2	X	93	TYR
2	X	96	ASP
2	X	100	GLU
2	X	104	GLU
2	X	106	LYS
2	X	113	PRO

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Mol	Chain	Res	Type
2	X	118	ASN
2	X	119	THR
2	X	133	LEU
2	X	140	ASP
2	X	141	ASP
2	X	142	LYS
2	X	143	PHE
2	X	163	ARG
2	X	166	LEU
2	X	168	LYS
2	X	179	ARG
2	X	187	PHE
2	X	211	ILE
2	X	215	LYS
2	X	217	ASN
2	X	219	LYS
2	X	221	LEU
2	X	222	ILE
2	X	229	PHE
2	X	230	LYS
2	X	263	GLN
2	X	267	LEU
2	X	274	ASN
2	X	278	VAL
2	X	279	GLN
2	X	280	GLU
2	X	281	LYS
2	X	282	LYS
2	X	283	LEU
2	X	284	LEU
2	X	292	SER
2	X	297	LYS
2	X	298	PHE
2	X	302	ILE
2	X	303	ASP
2	X	304	ASP
2	X	309	LEU
2	X	311	LEU
2	X	314	VAL
2	X	318	ILE
2	X	327	ARG
2	X	330	PHE

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Mol	Chain	Res	Type
2	X	331	LYS
2	X	334	GLU
2	X	340	LYS
2	X	341	PHE
2	X	359	GLN
2	X	383	THR
2	X	384	LEU
2	X	385	GLU
2	X	401	PHE
2	X	404	ILE
2	X	409	ARG
2	X	412	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	259	HIS
1	P	605	HIS
2	X	76	GLN
2	X	161	ASN
2	X	177	HIS
2	X	279	GLN
2	X	396	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GNP	P	1685	-	29,34,34	2.48	11 (37%)	28,54,54	1.86	7 (25%)

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	GNP	P	1685	-	-	0/16/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1685	GNP	C4-N9	-6.42	1.39	1.47
3	P	1685	GNP	C5-C6	-5.75	1.42	1.53
3	P	1685	GNP	PB-O3A	-4.51	1.53	1.59
3	P	1685	GNP	PB-O2B	-3.15	1.48	1.56
3	P	1685	GNP	PG-O2G	-3.12	1.48	1.56
3	P	1685	GNP	C8-N9	-2.91	1.37	1.47
3	P	1685	GNP	C2-N3	-2.28	1.33	1.43
3	P	1685	GNP	PB-O1B	2.21	1.48	1.46
3	P	1685	GNP	C1'-N9	2.65	1.47	1.42
3	P	1685	GNP	PG-O1G	3.32	1.49	1.46
3	P	1685	GNP	C6-N1	3.95	1.39	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1685	GNP	O3G-PG-O1G	-3.05	105.56	113.58
3	P	1685	GNP	O6-C6-N1	-2.27	119.82	122.80
3	P	1685	GNP	PA-O3A-PB	-2.14	124.94	132.71
3	P	1685	GNP	O3G-PG-O2G	3.12	116.73	107.67
3	P	1685	GNP	O2B-PB-O1B	3.69	117.29	110.02
3	P	1685	GNP	O6-C6-C5	4.43	128.16	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1685	GNP	C4-C5-N7	4.85	110.25	102.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1685	GNP	56	0

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.