



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 02:38 PM UTC

PDB ID : 4CRN / pdb_00004crn
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 Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

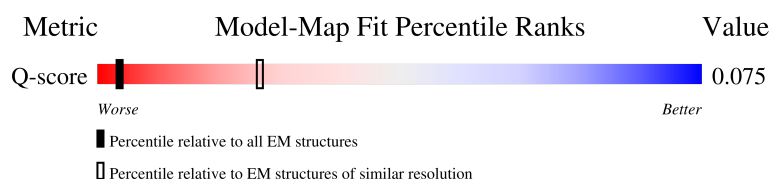
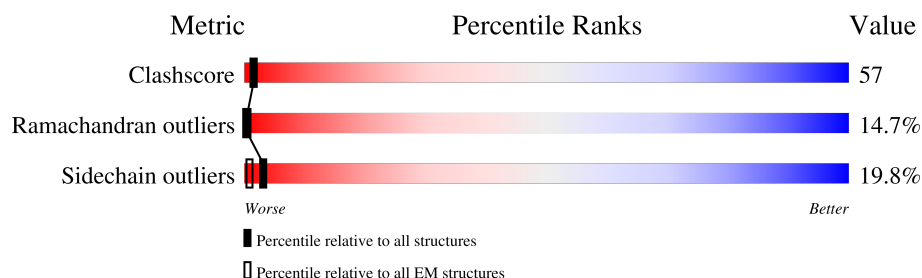
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	225 (8.70 - 9.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

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		

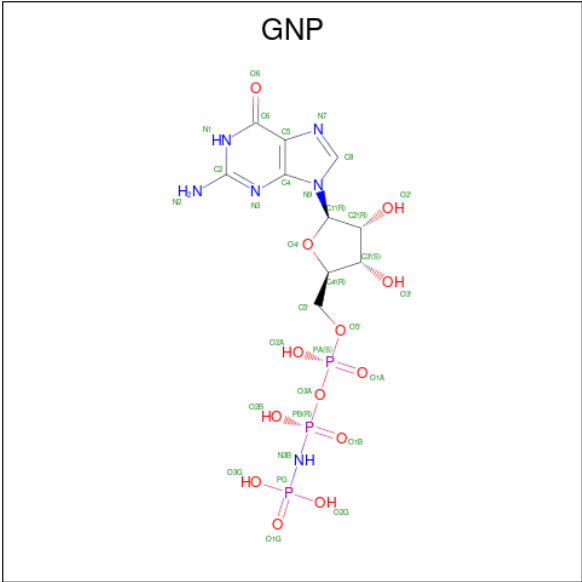
- Molecule 2 is a protein called ERF1 IN RIBOSOME-BOUND ERF1-ERF3-GDPNP COMPLEX.

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 (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

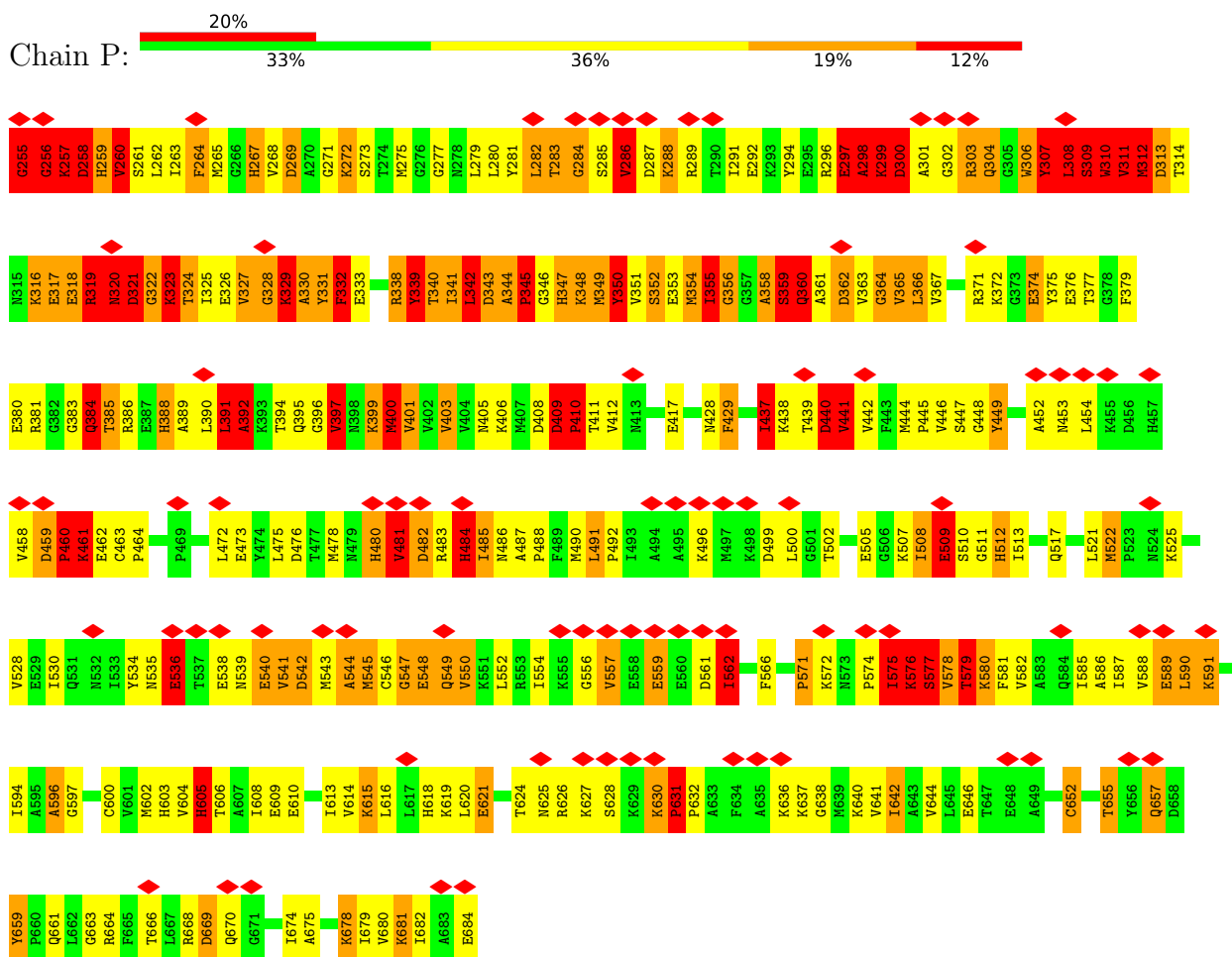


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	P	1	32	10	6	13	3	0

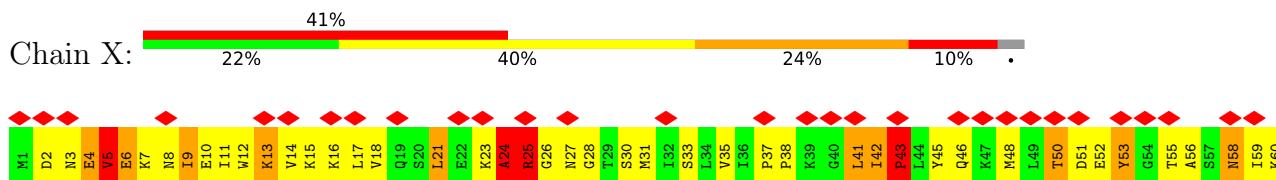
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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



ASP	V364	D304	A244	S183	Y122	S61
GLU	S365	T306	C245	A184	L123	R62
ASP	E366	L306	K246	L185	C124	V63
GLU	E367	K307	V247	R186	D125	R64
GLY	A308	A308	I248	F187	N126	R65
SER	P368	L309	S249	A188	K127	L66
ASP	L369	D310	I250	R189	F128	S67
ASP	T370	L311	V251	L190	H129	V68
ASP	E371	G312	D252	L191	T130	L69
ASP	V372	A313	V253	E192	E131	S70
PHE	L373	V314	S254	F193	V132	A71
ILE	A374	E315	Y255	K194	L136	I72
	A376	K316	G256	R195	L137	T73
	N376	L317	G257	H196	Q138	Q76
	V377	T318	E258	N197	A139	Q77
	K378	V319	N259	Y198	D140	K78
	N379	F320	G260	V199	D141	L79
	F380	E321	F261	K200	D142	K80
		N322	N262	R201	K142	L81
		L323	Q263	K202	F143	Y82
	T383	E324	A264	V202	G144	N83
	L384	T325	I265	A203	F145	T84
	E385	L326	E266	E204	V146	L85
	F386	R327	S267	V205	M147	P86
	L387	Y328	S268	V206	D148	K87
	T388	T329	A269	V207	D149	N88
	D389	F330	E270	Q208	G150	G89
	K390	K331	A271	N209	Q151	L90
	S391	D332	L272	F210	G152	V91
	S392	A333	A273	I211	T153	L92
	G394	E334	N274	T212	L154	Y93
	A395	D335	K275	N213	F155	C94
	Q396	D336	K276	D214	V158	G95
	F397	N336	V277	K215	S159	D96
	V398	E337	V278	V216	G160	I97
	T399	V338	E280	N217	N161	I98
	G400	T339	K281	V218	T162	T99
	F401	K340	K282	K219	R163	E100
	G402	F341	L283	G220	T164	D101
	G403	A342	L284	G221	V165	G102
	I404	E343	E285	L221	L166	K103
	G405	F344	A286	I222	H167	E104
	A406	A345	Y287	L223	K168	K105
	A407	A346	F288	D226	F169	K106
	L408	K347	D289	A227	T170	V107
	R409	D348	E290	D228	T171	T108
	Y410	K349	I291	F229	D172	F109
	K411	S350	Q292	K230	L173	D110
	V412	A352	D294	T231	P174	I111
	Q416	T295	T295	D232	K175	E112
	L417	G296	G296	L233	K176	P113
	L418	K297	K297	A234	G178	Y114
	V419	D354	K298	K235	R179	K115
	D420	K355	F298	S236	G180	P116
	E421	A356	C299	E237	G181	I117
	S421	T357	C300	L238	Q182	N118
	E422	G358	G301	F239		T119
	ASP	Q359	I302	D240		S120
GLU	K361	E360	D303	P241		L121
TYR	D362	K361		R242		
TYR	V363	V363		L243		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39309	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	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	147136	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	0.922	Depositor
Minimum map value	-0.456	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.183	Depositor
Map size ($\text{\AA}$)	455.4, 455.4, 455.4	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2375, 1.2375, 1.2375	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	P	1.26	19/3412 (0.6%)	2.17	159/4600 (3.5%)
2	X	2.57	70/3363 (2.1%)	3.06	285/4532 (6.3%)
All	All	2.02	89/6775 (1.3%)	2.65	444/9132 (4.9%)

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 (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	379	ASN	CG-ND2	97.10	3.37	1.33
2	X	183	SER	C-N	37.41	1.86	1.33
2	X	182	GLN	C-N	29.27	1.71	1.33
2	X	421	SER	C-N	-23.48	1.00	1.33
1	P	330	ALA	C-N	23.23	1.66	1.33
2	X	269	ALA	C-N	-16.93	1.09	1.33
2	X	368	PRO	CA-C	12.02	1.69	1.52
1	P	684	GLU	C-O	-11.57	1.00	1.23
2	X	421	SER	C-O	-11.57	1.00	1.23
2	X	37	PRO	CA-C	-10.35	1.42	1.52
2	X	342	ALA	C-N	10.07	1.54	1.33
2	X	42	ILE	CA-CB	9.96	1.60	1.53
1	P	545	MET	CA-C	-9.60	1.40	1.52
2	X	368	PRO	C-N	9.43	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	269	ALA	CA-C	8.94	1.64	1.52
2	X	279	GLN	CA-C	-8.77	1.41	1.52
2	X	161	ASN	CA-CB	8.65	1.64	1.53
2	X	269	ALA	N-CA	8.59	1.57	1.46
1	P	409	ASP	CG-OD1	-8.34	1.09	1.25
2	X	342	ALA	N-CA	-7.95	1.35	1.46
2	X	4	GLU	CA-C	-7.87	1.42	1.52
1	P	307	TYR	CA-C	7.71	1.64	1.53
2	X	196	HIS	ND1-CE1	7.53	1.40	1.32
2	X	95	GLY	CA-C	-7.44	1.42	1.51
2	X	174	PRO	N-CA	7.22	1.56	1.47
2	X	407	MET	CA-C	-7.08	1.44	1.53
2	X	17	LEU	N-CA	-7.06	1.37	1.46
1	P	308	LEU	N-CA	7.00	1.55	1.46
2	X	331	LYS	CA-C	-6.95	1.43	1.52
2	X	368	PRO	N-CA	6.87	1.56	1.47
2	X	43	PRO	CA-CB	-6.82	1.44	1.53
2	X	25	ARG	CA-C	-6.79	1.43	1.52
2	X	15	LYS	N-CA	-6.70	1.38	1.46
2	X	369	LEU	N-CA	6.69	1.55	1.46
1	P	323	LYS	N-CA	-6.58	1.37	1.46
2	X	86	PRO	CA-C	-6.58	1.45	1.53
1	P	259	HIS	CB-CG	6.52	1.59	1.50
2	X	62	ARG	CD-NE	6.44	1.55	1.46
1	P	256	GLY	CA-C	6.41	1.60	1.51
1	P	356	GLY	CA-C	-6.39	1.40	1.51
1	P	320	ASN	N-CA	-6.26	1.38	1.46
2	X	158	VAL	CA-C	-6.22	1.45	1.52
1	P	323	LYS	CA-C	-6.15	1.44	1.52
2	X	114	TYR	CA-CB	6.12	1.63	1.53
2	X	326	ILE	C-N	6.11	1.42	1.33
2	X	174	PRO	CA-C	5.99	1.60	1.52
2	X	299	CYS	C-N	-5.87	1.25	1.33
2	X	366	GLU	CA-C	5.87	1.60	1.52
2	X	192	GLU	CA-C	5.86	1.60	1.52
2	X	363	VAL	CA-CB	-5.84	1.46	1.54
2	X	145	PHE	CA-C	-5.82	1.45	1.52
2	X	53	TYR	CA-CB	5.81	1.62	1.53
2	X	340	LYS	C-N	5.78	1.41	1.33
1	P	317	GLU	CA-C	-5.78	1.45	1.52
2	X	341	PHE	CA-C	-5.74	1.45	1.52
2	X	152	GLY	CA-C	-5.69	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	369	LEU	CA-CB	5.69	1.61	1.52
2	X	276	LYS	N-CA	-5.62	1.39	1.46
2	X	173	LEU	CA-C	-5.61	1.46	1.52
1	P	324	THR	C-N	5.59	1.41	1.33
2	X	3	ASN	N-CA	-5.57	1.39	1.46
2	X	127	LYS	N-CA	-5.56	1.39	1.46
2	X	5	VAL	CA-C	5.56	1.59	1.52
1	P	345	PRO	CA-C	-5.55	1.44	1.52
2	X	144	GLY	CA-C	-5.54	1.48	1.52
2	X	90	LEU	CA-C	-5.46	1.45	1.52
2	X	203	ALA	C-N	5.38	1.41	1.33
2	X	386	PHE	C-N	5.37	1.41	1.33
2	X	349	LYS	CA-C	-5.31	1.45	1.52
1	P	349	MET	SD-CE	-5.31	1.66	1.79
1	P	321	ASP	CA-CB	5.28	1.62	1.53
2	X	171	VAL	N-CA	-5.28	1.40	1.46
2	X	410	TYR	CA-C	-5.24	1.46	1.52
2	X	223	LEU	CA-CB	5.24	1.60	1.53
2	X	279	GLN	CA-CB	5.23	1.62	1.53
2	X	55	THR	CA-C	-5.23	1.46	1.52
2	X	364	VAL	N-CA	-5.17	1.39	1.46
2	X	291	ILE	CA-C	-5.17	1.45	1.52
2	X	3	ASN	CA-C	-5.16	1.46	1.52
1	P	338	ARG	CA-C	-5.12	1.46	1.52
1	P	331	TYR	C-N	5.10	1.39	1.33
2	X	252	ASP	C-O	-5.10	1.17	1.24
2	X	140	ASP	CA-C	-5.08	1.46	1.52
2	X	200	ARG	CA-C	5.08	1.59	1.52
2	X	342	ALA	CA-C	5.08	1.59	1.52
2	X	283	LEU	C-N	5.07	1.40	1.33
2	X	364	VAL	CA-CB	-5.07	1.47	1.54
2	X	5	VAL	C-N	5.06	1.41	1.34
2	X	260	GLY	N-CA	-5.02	1.39	1.45

All (444) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	379	ASN	OD1-CG-ND2	-103.21	19.39	122.60
2	X	183	SER	O-C-N	31.26	159.49	122.92
2	X	269	ALA	O-C-N	-29.58	83.25	122.59
1	P	320	ASN	CA-C-N	18.20	156.31	121.54
1	P	320	ASN	C-N-CA	18.20	156.31	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	367	GLU	CA-C-O	-17.72	99.67	120.05
2	X	183	SER	CA-C-N	-16.23	90.55	121.54
2	X	183	SER	C-N-CA	-16.23	90.55	121.54
1	P	330	ALA	O-C-N	15.32	138.97	123.04
1	P	321	ASP	N-CA-C	15.21	143.19	110.80
1	P	545	MET	CG-SD-CE	15.13	134.19	100.90
2	X	173	LEU	O-C-N	-14.91	93.88	120.56
2	X	369	LEU	CB-CA-C	-13.87	88.51	111.68
2	X	174	PRO	CB-CA-C	-13.81	88.77	111.56
2	X	341	PHE	CA-CB-CG	13.77	127.57	113.80
2	X	299	CYS	CA-C-N	13.66	142.54	122.87
2	X	299	CYS	C-N-CA	13.66	142.54	122.87
2	X	3	ASN	N-CA-C	-13.51	86.50	108.52
2	X	302	ILE	N-CA-C	13.50	124.85	112.43
2	X	177	HIS	CA-CB-CG	13.46	127.26	113.80
2	X	405	GLY	O-C-N	-13.27	111.55	123.36
2	X	14	VAL	CA-C-N	12.76	137.37	120.28
2	X	14	VAL	C-N-CA	12.76	137.37	120.28
2	X	291	ILE	CB-CA-C	-12.67	92.52	112.16
2	X	161	ASN	N-CA-C	-12.64	95.58	112.26
2	X	41	LEU	CA-C-N	12.48	128.10	120.24
2	X	41	LEU	C-N-CA	12.48	128.10	120.24
2	X	182	GLN	CA-C-N	-12.24	102.65	122.11
2	X	182	GLN	C-N-CA	-12.24	102.65	122.11
2	X	15	LYS	CB-CA-C	12.19	131.03	110.79
2	X	142	LYS	N-CA-CB	11.96	130.71	110.49
2	X	421	SER	O-C-N	11.87	141.99	123.00
2	X	281	LYS	CA-C-N	11.80	144.08	121.54
2	X	281	LYS	C-N-CA	11.80	144.08	121.54
2	X	145	PHE	CA-CB-CG	-11.54	102.26	113.80
1	P	321	ASP	CB-CA-C	-11.42	87.69	110.42
1	P	379	PHE	CA-C-N	11.40	143.32	121.54
1	P	379	PHE	C-N-CA	11.40	143.32	121.54
2	X	273	ALA	CA-C-N	11.17	142.88	121.54
2	X	273	ALA	C-N-CA	11.17	142.88	121.54
2	X	341	PHE	N-CA-CB	10.58	128.37	110.49
1	P	380	GLU	N-CA-C	-10.51	88.42	110.80
2	X	404	ILE	CA-C-N	10.37	131.31	121.46
2	X	404	ILE	C-N-CA	10.37	131.31	121.46
1	P	324	THR	CA-C-N	-10.19	112.78	123.08
1	P	324	THR	C-N-CA	-10.19	112.78	123.08
1	P	318	GLU	O-C-N	-10.16	109.08	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	316	LYS	CB-CA-C	-10.04	92.06	110.63
2	X	209	ASN	CA-C-N	10.02	133.47	120.44
2	X	209	ASN	C-N-CA	10.02	133.47	120.44
1	P	400	MET	CB-CA-C	9.97	130.26	110.42
2	X	379	ASN	CB-CG-ND2	-9.92	101.52	116.40
2	X	5	VAL	CB-CA-C	9.88	127.50	111.29
2	X	284	LEU	CB-CA-C	-9.86	95.04	110.81
2	X	396	GLN	CB-CA-C	-9.85	94.11	110.85
2	X	186	ARG	CB-CA-C	-9.70	91.12	110.42
2	X	4	GLU	N-CA-C	-9.63	94.69	109.24
2	X	292	SER	O-C-N	-9.47	110.08	122.39
1	P	545	MET	CA-CB-CG	9.47	133.03	114.10
2	X	13	LYS	CA-C-N	9.45	133.40	120.46
2	X	13	LYS	C-N-CA	9.45	133.40	120.46
2	X	84	THR	N-CA-CB	9.44	127.42	111.66
2	X	331	LYS	N-CA-CB	9.39	126.17	111.24
2	X	211	ILE	CB-CA-C	9.33	123.31	112.68
2	X	50	THR	N-CA-C	9.31	121.43	111.28
2	X	84	THR	N-CA-C	-9.26	94.99	109.07
2	X	9	ILE	N-CA-CB	9.26	124.47	110.58
1	P	258	ASP	CA-CB-CG	-9.07	103.53	112.60
2	X	16	LYS	CB-CA-C	-9.03	96.70	110.88
2	X	277	TYR	CA-C-N	8.80	133.52	122.43
2	X	277	TYR	C-N-CA	8.80	133.52	122.43
2	X	369	LEU	N-CA-CB	8.77	125.09	110.53
1	P	348	LYS	CB-CA-C	-8.74	93.58	113.33
2	X	201	LYS	N-CA-C	8.72	120.78	111.28
1	P	307	TYR	N-CA-C	8.64	124.13	107.71
1	P	338	ARG	N-CA-CB	8.57	124.05	110.85
2	X	174	PRO	CA-N-CD	-8.55	100.03	112.00
2	X	300	PHE	N-CA-C	8.39	121.04	109.54
1	P	347	HIS	CA-CB-CG	8.39	122.19	113.80
1	P	306	TRP	CB-CA-C	8.33	123.47	110.14
1	P	631	PRO	N-CA-C	8.25	120.76	110.70
1	P	317	GLU	N-CA-CB	8.19	121.87	109.91
2	X	9	ILE	O-C-N	-8.19	113.40	121.83
2	X	174	PRO	O-C-N	-8.19	111.58	122.64
2	X	368	PRO	CA-C-N	8.18	134.87	122.77
2	X	368	PRO	C-N-CA	8.18	134.87	122.77
2	X	273	ALA	N-CA-C	-8.14	93.47	110.80
2	X	227	ALA	N-CA-CB	-8.13	99.67	111.70
2	X	281	LYS	CB-CA-C	8.06	126.47	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	290	GLU	CB-CA-C	8.04	124.14	110.79
2	X	143	PHE	CA-CB-CG	8.02	121.82	113.80
2	X	9	ILE	CB-CA-C	-7.99	101.20	112.22
2	X	137	LEU	N-CA-C	-7.97	90.85	107.67
2	X	172	ASP	N-CA-C	-7.91	95.52	108.41
2	X	177	HIS	CA-C-N	7.88	136.86	121.41
2	X	177	HIS	C-N-CA	7.88	136.86	121.41
2	X	42	ILE	CA-C-N	7.87	127.59	119.56
2	X	42	ILE	C-N-CA	7.87	127.59	119.56
2	X	227	ALA	CA-C-N	7.86	135.50	123.47
2	X	227	ALA	C-N-CA	7.86	135.50	123.47
2	X	11	ILE	CA-C-N	7.86	130.66	120.44
2	X	11	ILE	C-N-CA	7.86	130.66	120.44
2	X	33	SER	N-CA-CB	7.83	123.33	110.17
1	P	259	HIS	CB-CA-C	7.83	122.05	110.62
2	X	248	ILE	N-CA-CB	7.83	121.79	110.52
1	P	544	ALA	CA-C-N	7.75	135.57	121.85
1	P	544	ALA	C-N-CA	7.75	135.57	121.85
1	P	441	VAL	N-CA-CB	7.75	124.01	111.23
1	P	320	ASN	O-C-N	7.71	132.84	122.59
1	P	578	VAL	CA-C-N	7.70	136.25	121.54
1	P	578	VAL	C-N-CA	7.70	136.25	121.54
2	X	363	VAL	CA-C-N	7.69	135.81	121.97
2	X	363	VAL	C-N-CA	7.69	135.81	121.97
2	X	269	ALA	N-CA-C	7.66	127.11	110.80
2	X	226	SER	CB-CA-C	-7.66	96.08	109.86
1	P	257	LYS	N-CA-CB	7.65	123.19	111.56
2	X	220	GLY	N-CA-C	7.63	131.26	113.18
2	X	83	ASN	CB-CA-C	7.62	123.80	110.85
2	X	330	PHE	O-C-N	-7.60	112.49	122.59
2	X	6	GLU	CB-CA-C	-7.58	96.13	110.67
1	P	302	GLY	CA-C-N	7.57	135.99	121.54
1	P	302	GLY	C-N-CA	7.57	135.99	121.54
2	X	240	ASP	CA-CB-CG	7.55	120.15	112.60
1	P	562	ILE	CA-CB-CG1	7.55	123.23	110.40
2	X	367	GLU	O-C-N	-7.55	111.96	121.70
2	X	135	GLU	CA-C-N	7.54	131.76	120.31
2	X	135	GLU	C-N-CA	7.54	131.76	120.31
2	X	265	ILE	CB-CA-C	-7.53	98.94	111.29
1	P	321	ASP	N-CA-CB	-7.51	97.80	110.49
1	P	480	HIS	CA-C-N	7.50	135.46	121.97
1	P	480	HIS	C-N-CA	7.50	135.46	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	279	GLN	N-CA-CB	7.49	123.15	110.49
1	P	384	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	P	297	GLU	CA-C-N	7.47	135.81	121.54
1	P	297	GLU	C-N-CA	7.47	135.81	121.54
1	P	348	LYS	CG-CD-CE	7.47	128.47	111.30
1	P	545	MET	CB-CA-C	-7.46	94.05	109.94
2	X	85	LEU	N-CA-CB	-7.44	96.06	109.68
2	X	404	ILE	O-C-N	-7.44	114.47	123.03
2	X	246	LYS	N-CA-C	7.43	122.17	113.18
1	P	349	MET	CB-CA-C	-7.39	97.68	110.17
2	X	365	SER	CA-C-N	7.39	135.66	121.54
2	X	365	SER	C-N-CA	7.39	135.66	121.54
1	P	308	LEU	N-CA-C	7.37	126.49	110.80
1	P	481	VAL	CA-CB-CG2	7.35	122.89	110.40
2	X	25	ARG	CA-C-N	7.33	135.78	121.41
2	X	25	ARG	C-N-CA	7.33	135.78	121.41
1	P	362	ASP	CA-CB-CG	7.32	119.92	112.60
1	P	657	GLN	OE1-CD-NE2	-7.27	115.33	122.60
2	X	342	ALA	CA-C-N	-7.25	104.10	121.80
2	X	342	ALA	C-N-CA	-7.25	104.10	121.80
1	P	329	LYS	N-CA-C	7.17	120.46	108.13
2	X	158	VAL	N-CA-CB	7.17	121.30	111.41
2	X	252	ASP	CA-CB-CG	-7.14	105.46	112.60
2	X	283	LEU	CA-C-O	-7.14	111.92	120.56
2	X	412	VAL	CA-C-N	7.14	131.63	121.42
2	X	412	VAL	C-N-CA	7.14	131.63	121.42
2	X	162	THR	O-C-N	-7.12	114.16	123.13
2	X	41	LEU	N-CA-CB	7.10	122.12	110.69
1	P	255	GLY	CA-C-N	7.08	135.29	121.41
1	P	255	GLY	C-N-CA	7.08	135.29	121.41
2	X	219	LYS	CB-CA-C	7.08	123.32	109.72
1	P	499	ASP	CA-CB-CG	6.98	119.58	112.60
2	X	84	THR	CB-CA-C	-6.97	95.46	110.45
2	X	421	SER	CA-C-O	-6.94	109.00	120.80
2	X	23	LYS	N-CA-C	-6.92	100.98	111.56
1	P	257	LYS	CB-CG-CD	6.88	127.13	111.30
1	P	596	ALA	CA-C-N	6.86	133.10	122.20
1	P	596	ALA	C-N-CA	6.86	133.10	122.20
2	X	342	ALA	N-CA-CB	-6.86	98.91	110.49
2	X	27	ASN	CA-CB-CG	6.85	119.45	112.60
1	P	320	ASN	CA-C-O	6.85	130.30	120.51
2	X	244	ALA	CA-C-N	6.84	130.00	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	244	ALA	C-N-CA	6.84	130.00	120.29
2	X	339	ILE	CB-CA-C	6.82	120.59	110.98
1	P	322	GLY	CA-C-N	6.79	134.88	122.79
1	P	322	GLY	C-N-CA	6.79	134.88	122.79
2	X	277	TYR	CB-CA-C	-6.79	101.92	112.31
2	X	63	VAL	N-CA-C	6.78	116.92	110.42
1	P	299	LYS	CG-CD-CE	6.77	126.86	111.30
2	X	342	ALA	CB-CA-C	6.75	123.86	110.42
1	P	303	ARG	N-CA-CB	-6.73	99.12	110.49
1	P	517	GLN	OE1-CD-NE2	-6.72	115.88	122.60
2	X	21	LEU	CB-CA-C	-6.72	100.28	110.90
1	P	300	ASP	CA-C-N	6.69	133.63	121.06
1	P	300	ASP	C-N-CA	6.69	133.63	121.06
1	P	316	LYS	N-CA-CB	6.65	120.46	110.22
2	X	8	ASN	N-CA-C	6.63	120.63	112.54
2	X	83	ASN	CA-C-N	6.63	133.22	121.75
2	X	83	ASN	C-N-CA	6.63	133.22	121.75
2	X	51	ASP	CA-CB-CG	6.62	119.22	112.60
2	X	158	VAL	N-CA-C	-6.60	98.86	108.11
1	P	360	GLN	OE1-CD-NE2	-6.60	116.00	122.60
2	X	342	ALA	CA-C-O	-6.54	111.16	120.51
2	X	175	LYS	N-CA-C	-6.53	105.45	113.41
2	X	16	LYS	N-CA-CB	-6.49	100.60	110.01
2	X	16	LYS	CA-C-N	6.49	128.97	120.28
2	X	16	LYS	C-N-CA	6.49	128.97	120.28
1	P	484	HIS	CA-C-N	6.48	133.64	121.97
1	P	484	HIS	C-N-CA	6.48	133.64	121.97
2	X	291	ILE	CB-CG1-CD1	-6.48	100.19	113.80
2	X	299	CYS	O-C-N	-6.48	115.64	123.29
2	X	78	LYS	CA-C-O	-6.47	113.56	120.42
2	X	366	GLU	CA-C-N	6.46	146.10	121.95
2	X	366	GLU	C-N-CA	6.46	146.10	121.95
2	X	248	ILE	CB-CA-C	-6.44	103.60	112.04
2	X	6	GLU	CA-C-N	6.44	128.91	120.28
2	X	6	GLU	C-N-CA	6.44	128.91	120.28
2	X	161	ASN	O-C-N	-6.43	113.97	122.20
1	P	324	THR	CA-C-O	-6.42	112.30	120.14
1	P	320	ASN	CB-CA-C	6.39	123.14	110.42
2	X	292	SER	CA-C-N	-6.38	112.06	122.65
2	X	292	SER	C-N-CA	-6.38	112.06	122.65
2	X	264	ALA	N-CA-CB	6.37	121.25	110.49
2	X	247	VAL	O-C-N	-6.35	115.53	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	311	VAL	CB-CA-C	6.35	121.70	111.29
2	X	297	LYS	N-CA-C	-6.34	104.70	112.88
2	X	166	LEU	O-C-N	-6.33	114.17	122.59
1	P	350	TYR	CA-CB-CG	6.32	125.27	113.90
1	P	308	LEU	CA-C-N	6.32	133.60	121.54
1	P	308	LEU	C-N-CA	6.32	133.60	121.54
1	P	306	TRP	CA-C-N	6.29	133.69	123.37
1	P	306	TRP	C-N-CA	6.29	133.69	123.37
2	X	9	ILE	CA-C-O	6.28	127.50	120.85
2	X	349	LYS	N-CA-CB	6.27	121.08	110.49
1	P	545	MET	N-CA-CB	6.26	123.17	111.52
2	X	407	MET	CB-CA-C	-6.25	103.20	111.82
2	X	79	LEU	N-CA-CB	-6.23	100.62	110.22
1	P	344	ALA	CA-C-N	6.22	127.61	119.84
1	P	344	ALA	C-N-CA	6.22	127.61	119.84
1	P	388	HIS	CA-CB-CG	6.21	120.01	113.80
1	P	484	HIS	CA-C-O	-6.20	114.75	121.44
2	X	293	GLN	CA-C-N	6.19	133.37	121.54
2	X	293	GLN	C-N-CA	6.19	133.37	121.54
2	X	115	LYS	N-CA-C	6.18	123.46	109.81
2	X	163	ARG	CB-CA-C	6.17	120.48	109.38
1	P	257	LYS	CA-C-N	6.16	133.31	121.54
1	P	257	LYS	C-N-CA	6.16	133.31	121.54
2	X	24	ALA	N-CA-CB	6.14	121.43	112.28
2	X	18	VAL	CB-CA-C	-6.14	103.85	112.14
2	X	325	THR	N-CA-CB	6.13	121.50	110.83
2	X	41	LEU	CB-CA-C	6.12	120.40	109.38
2	X	228	ASP	CA-CB-CG	-6.12	106.48	112.60
2	X	276	LYS	N-CA-CB	-6.10	100.18	110.49
1	P	350	TYR	CG-CD2-CE2	-6.10	112.05	121.20
2	X	24	ALA	CA-C-N	6.10	133.19	121.54
2	X	24	ALA	C-N-CA	6.10	133.19	121.54
2	X	261	PHE	CA-CB-CG	-6.08	107.72	113.80
1	P	460	PRO	CA-C-N	6.07	133.13	121.54
1	P	460	PRO	C-N-CA	6.07	133.13	121.54
2	X	42	ILE	N-CA-CB	-6.06	106.68	110.50
1	P	319	ARG	O-C-N	-6.04	115.09	122.34
2	X	177	HIS	CB-CA-C	-6.03	96.67	110.18
2	X	93	TYR	CB-CG-CD1	6.01	129.82	120.80
2	X	272	LEU	CA-C-N	6.01	133.03	121.54
2	X	272	LEU	C-N-CA	6.01	133.03	121.54
2	X	171	VAL	CA-C-N	-6.01	114.52	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	171	VAL	C-N-CA	-6.01	114.52	123.00
1	P	410	PRO	CA-C-N	6.00	133.00	121.54
1	P	410	PRO	C-N-CA	6.00	133.00	121.54
2	X	92	LEU	CA-C-O	5.99	127.64	120.28
1	P	559	GLU	CA-C-N	5.98	129.11	120.38
1	P	559	GLU	C-N-CA	5.98	129.11	120.38
2	X	137	LEU	CA-C-N	5.96	132.93	121.54
2	X	137	LEU	C-N-CA	5.96	132.93	121.54
1	P	255	GLY	CA-C-O	-5.96	108.28	120.80
2	X	243	LEU	N-CA-C	5.96	117.85	111.36
2	X	173	LEU	N-CA-C	-5.94	100.32	109.41
2	X	161	ASN	CB-CA-C	-5.94	101.57	111.13
1	P	319	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	P	338	ARG	N-CA-C	-5.92	100.96	110.14
2	X	386	PHE	CA-C-O	-5.91	114.89	121.51
2	X	139	ALA	N-CA-CB	5.88	120.42	110.49
1	P	384	GLN	CA-C-N	5.87	128.63	120.29
1	P	384	GLN	C-N-CA	5.87	128.63	120.29
2	X	73	THR	N-CA-CB	5.86	118.74	110.12
2	X	166	LEU	CA-C-O	5.86	128.89	120.51
2	X	369	LEU	O-C-N	5.85	129.77	122.63
2	X	298	PHE	N-CA-CB	5.85	119.74	110.55
2	X	27	ASN	CA-C-N	5.85	132.87	121.41
2	X	27	ASN	C-N-CA	5.85	132.87	121.41
1	P	283	THR	CA-C-N	5.84	127.49	120.13
1	P	283	THR	C-N-CA	5.84	127.49	120.13
2	X	369	LEU	CA-C-N	5.84	132.49	121.97
2	X	369	LEU	C-N-CA	5.84	132.49	121.97
2	X	232	ASP	CA-C-O	5.84	126.64	119.05
2	X	278	VAL	CA-C-O	-5.83	113.64	120.75
1	P	307	TYR	O-C-N	-5.82	115.26	122.82
1	P	605	HIS	CE1-NE2-CD2	-5.81	103.19	109.00
2	X	77	GLN	N-CA-C	5.80	117.61	111.28
2	X	56	ALA	CA-C-N	5.80	128.64	120.28
2	X	56	ALA	C-N-CA	5.80	128.64	120.28
1	P	509	GLU	CB-CA-C	-5.79	100.11	110.70
1	P	259	HIS	CA-C-N	5.78	132.37	121.97
1	P	259	HIS	C-N-CA	5.78	132.37	121.97
1	P	359	SER	N-CA-C	5.78	123.10	110.80
1	P	670	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	P	379	PHE	N-CA-C	-5.75	98.54	110.80
2	X	337	GLU	CB-CA-C	5.75	120.36	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	284	GLY	CA-C-N	5.75	132.52	121.54
1	P	284	GLY	C-N-CA	5.75	132.52	121.54
2	X	240	ASP	N-CA-C	5.74	122.50	109.81
2	X	331	LYS	CB-CG-CD	5.74	124.51	111.30
1	P	256	GLY	O-C-N	-5.74	115.24	122.70
1	P	682	ILE	N-CA-CB	-5.74	102.64	110.56
2	X	167	HIS	N-CA-CB	5.74	120.19	110.49
2	X	43	PRO	N-CA-CB	5.73	109.21	103.48
2	X	51	ASP	N-CA-C	5.72	117.60	111.36
2	X	51	ASP	CB-CG-OD2	-5.72	105.24	118.40
1	P	391	LEU	CA-C-N	5.72	132.47	121.54
1	P	391	LEU	C-N-CA	5.72	132.47	121.54
1	P	508	ILE	CB-CA-C	5.72	119.35	110.83
2	X	326	ILE	CA-CB-CG2	-5.71	100.79	110.50
2	X	341	PHE	CB-CA-C	-5.71	99.06	110.42
2	X	232	ASP	O-C-N	-5.70	114.59	122.46
1	P	400	MET	CA-CB-CG	5.70	125.49	114.10
2	X	205	VAL	CA-C-O	5.69	126.90	119.85
2	X	331	LYS	CG-CD-CE	5.68	124.37	111.30
1	P	576	LYS	CA-C-O	-5.68	115.34	121.36
1	P	355	ILE	CB-CG1-CD1	5.68	125.72	113.80
1	P	350	TYR	CB-CG-CD2	-5.67	112.29	120.80
1	P	571	PRO	CA-C-N	5.66	132.34	121.54
1	P	571	PRO	C-N-CA	5.66	132.34	121.54
2	X	368	PRO	N-CA-CB	-5.65	97.31	103.25
1	P	267	HIS	CA-CB-CG	5.65	119.45	113.80
1	P	307	TYR	CA-C-N	5.65	132.33	121.54
1	P	307	TYR	C-N-CA	5.65	132.33	121.54
1	P	256	GLY	N-CA-C	5.64	126.56	113.18
2	X	25	ARG	CA-C-O	-5.64	112.44	120.51
1	P	365	VAL	N-CA-CB	5.64	118.80	111.19
2	X	158	VAL	CB-CA-C	5.64	118.97	110.63
2	X	48	MET	O-C-N	-5.63	116.15	122.12
2	X	6	GLU	N-CA-CB	5.63	119.01	110.28
2	X	299	CYS	CA-C-O	5.63	126.51	120.38
2	X	43	PRO	CA-N-CD	-5.61	104.15	112.00
1	P	298	ALA	N-CA-C	5.61	122.74	110.80
1	P	577	SER	N-CA-C	5.58	116.95	108.07
1	P	299	LYS	CA-C-N	5.58	132.19	121.54
1	P	299	LYS	C-N-CA	5.58	132.19	121.54
2	X	17	LEU	CB-CA-C	5.58	120.05	110.79
2	X	209	ASN	CA-CB-CG	5.58	118.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	405	GLY	CA-C-N	5.57	132.18	122.82
2	X	405	GLY	C-N-CA	5.57	132.18	122.82
1	P	286	VAL	CA-CB-CG2	5.57	119.86	110.40
2	X	59	ILE	N-CA-C	5.57	116.97	110.62
2	X	15	LYS	CA-C-N	-5.56	113.21	120.44
2	X	15	LYS	C-N-CA	-5.56	113.21	120.44
2	X	292	SER	N-CA-C	-5.56	105.59	112.38
1	P	681	LYS	CA-C-N	5.56	131.39	122.50
1	P	681	LYS	C-N-CA	5.56	131.39	122.50
1	P	316	LYS	CG-CD-CE	5.54	124.05	111.30
2	X	126	ASN	O-C-N	5.52	129.73	122.33
1	P	307	TYR	N-CA-CB	-5.52	96.85	110.32
2	X	159	SER	N-CA-CB	-5.51	102.27	110.71
2	X	112	GLU	CB-CA-C	-5.51	103.82	110.15
2	X	253	VAL	CB-CA-C	5.50	118.73	111.19
2	X	279	GLN	CA-CB-CG	5.50	125.10	114.10
2	X	279	GLN	N-CA-C	-5.50	99.09	110.80
2	X	323	LEU	CA-C-N	5.49	131.61	122.66
2	X	323	LEU	C-N-CA	5.49	131.61	122.66
2	X	113	PRO	CB-CA-C	5.49	120.61	111.56
2	X	10	GLU	CA-C-O	5.46	126.34	120.55
2	X	159	SER	N-CA-C	-5.46	98.11	107.61
2	X	135	GLU	N-CA-CB	5.45	118.22	110.16
2	X	263	GLN	N-CA-C	-5.42	104.77	111.33
1	P	459	ASP	CA-C-N	5.42	125.07	119.05
1	P	459	ASP	C-N-CA	5.42	125.07	119.05
2	X	281	LYS	CA-C-O	-5.40	112.78	120.51
1	P	397	VAL	CG1-CB-CG2	-5.39	98.93	110.80
2	X	82	TYR	CA-C-N	5.39	127.95	120.29
2	X	82	TYR	C-N-CA	5.39	127.95	120.29
1	P	319	ARG	CG-CD-NE	-5.39	100.15	112.00
1	P	339	TYR	N-CA-C	-5.36	99.70	108.76
2	X	56	ALA	CA-C-O	5.36	126.15	120.10
2	X	60	LYS	CB-CG-CD	5.36	123.62	111.30
2	X	250	ILE	N-CA-CB	5.33	118.62	111.90
1	P	605	HIS	ND1-CE1-NE2	5.32	113.72	108.40
2	X	55	THR	N-CA-C	5.32	117.08	111.28
2	X	223	LEU	CB-CA-C	-5.32	101.57	110.19
2	X	363	VAL	CA-CB-CG2	-5.31	101.37	110.40
1	P	259	HIS	CG-CD2-NE2	5.30	112.50	107.20
2	X	146	ILE	N-CA-CB	5.29	119.01	111.82
2	X	5	VAL	CA-CB-CG2	5.28	119.37	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	291	ILE	CA-CB-CG2	5.27	119.46	110.50
1	P	319	ARG	CD-NE-CZ	-5.27	117.03	124.40
2	X	262	ASN	N-CA-CB	5.25	117.63	110.01
2	X	182	GLN	CB-CA-C	-5.25	110.09	117.23
1	P	298	ALA	CA-C-N	-5.24	114.63	122.39
1	P	298	ALA	C-N-CA	-5.24	114.63	122.39
1	P	332	PHE	N-CA-C	5.23	115.04	108.45
2	X	83	ASN	N-CA-C	5.23	117.06	111.36
2	X	68	VAL	O-C-N	-5.22	116.80	121.87
2	X	51	ASP	CB-CG-OD1	5.22	130.40	118.40
2	X	43	PRO	CA-CB-CG	-5.21	94.60	104.50
1	P	317	GLU	N-CA-C	-5.21	105.30	110.97
1	P	342	LEU	CB-CA-C	5.20	118.64	109.80
2	X	195	ARG	NE-CZ-NH1	5.20	126.70	121.50
2	X	364	VAL	CB-CA-C	5.20	119.82	111.29
1	P	299	LYS	N-CA-C	5.20	116.89	108.26
2	X	301	GLY	N-CA-C	5.20	125.49	113.18
2	X	76	GLN	CB-CA-C	-5.18	102.19	110.79
1	P	304	GLN	N-CA-C	-5.18	106.81	113.23
2	X	409	ARG	CA-C-N	5.17	132.02	122.92
2	X	409	ARG	C-N-CA	5.17	132.02	122.92
2	X	340	LYS	CA-C-N	5.17	131.41	121.54
2	X	340	LYS	C-N-CA	5.17	131.41	121.54
2	X	37	PRO	N-CA-C	5.16	117.00	110.70
2	X	10	GLU	N-CA-C	5.16	116.90	111.28
1	P	318	GLU	CA-C-N	-5.16	114.40	122.65
1	P	318	GLU	C-N-CA	-5.16	114.40	122.65
1	P	396	GLY	CA-C-O	-5.15	116.61	121.87
1	P	320	ASN	CA-CB-CG	5.14	117.75	112.60
2	X	128	PHE	O-C-N	-5.14	117.36	123.22
2	X	341	PHE	CB-CG-CD1	5.14	129.44	120.70
1	P	536	GLU	N-CA-CB	-5.14	101.80	110.49
2	X	340	LYS	CA-C-O	-5.14	114.83	120.43
2	X	190	LEU	O-C-N	-5.13	116.21	122.22
2	X	18	VAL	N-CA-C	5.13	115.85	110.62
2	X	149	ASP	CA-C-N	5.12	125.63	120.00
2	X	149	ASP	C-N-CA	5.12	125.63	120.00
2	X	127	LYS	CA-C-N	5.12	129.41	122.19
2	X	127	LYS	C-N-CA	5.12	129.41	122.19
1	P	282	LEU	CA-C-N	5.11	128.49	120.82
1	P	282	LEU	C-N-CA	5.11	128.49	120.82
1	P	491	LEU	CA-C-N	5.11	124.86	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	491	LEU	C-N-CA	5.11	124.86	119.76
2	X	163	ARG	N-CA-C	-5.10	101.38	109.59
2	X	195	ARG	N-CA-CB	5.09	117.69	110.16
2	X	137	LEU	N-CA-CB	5.09	119.82	111.58
2	X	84	THR	CA-CB-OG1	5.08	117.22	109.60
2	X	216	VAL	N-CA-CB	-5.08	104.06	110.31
2	X	268	SER	CA-C-O	-5.08	113.25	120.51
2	X	274	ASN	CA-CB-CG	-5.08	107.52	112.60
2	X	242	ARG	CA-C-N	5.06	127.48	120.29
2	X	242	ARG	C-N-CA	5.06	127.48	120.29
2	X	284	LEU	N-CA-CB	5.05	117.46	109.94
1	P	627	LYS	O-C-N	5.05	127.28	122.03
2	X	58	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	P	540	GLU	CA-C-N	5.04	131.04	121.97
1	P	540	GLU	C-N-CA	5.04	131.04	121.97
2	X	76	GLN	CA-C-O	5.03	125.88	120.55
2	X	71	ALA	N-CA-C	5.02	116.56	111.14
1	P	299	LYS	CB-CG-CD	5.01	122.82	111.30
2	X	192	GLU	N-CA-C	5.00	118.65	112.54

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	Mainchain,Sidechain
1	P	298	ALA	Peptide
1	P	299	LYS	Peptide
1	P	300	ASP	Peptide

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Mol	Chain	Res	Type	Group
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	Peptide,Sidechain
1	P	321	ASP	Peptide
1	P	339	TYR	Peptide,Sidechain
1	P	340	THR	Peptide,Mainchain
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	Peptide,Mainchain
1	P	359	SER	Mainchain
1	P	360	GLN	Sidechain
1	P	362	ASP	Mainchain,Sidechain
1	P	364	GLY	Peptide,Mainchain
1	P	374	GLU	Sidechain
1	P	376	GLU	Mainchain
1	P	385	THR	Peptide,Mainchain
1	P	390	LEU	Peptide
1	P	391	LEU	Peptide
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	Peptide,Mainchain
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

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Mol	Chain	Res	Type	Group
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	Peptide,Sidechain
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	Peptide,Mainchain
1	P	631	PRO	Mainchain
1	P	632	PRO	Peptide
1	P	646	GLU	Sidechain
1	P	657	GLN	Sidechain
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

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Mol	Chain	Res	Type	Group
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 [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	P	3351	0	3391	346	0
2	X	3310	0	3338	440	0
3	P	32	0	12	56	0
All	All	6693	0	6741	769	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 57.

All (769) 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:182:GLN:C	2:X:183:SER:N	1.71	1.45
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
1:P:331:TYR:OH	1:P:536:GLU:C	1.63	1.41
2:X:161:ASN:ND2	2:X:390:LYS:HB2	1.18	1.41
2:X:354:ASP:HB3	2:X:357:THR:CG2	1.50	1.39
1:P:271:GLY:HA3	3:P:1685:GNP:C8	1.51	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:354:ASP:HB2	2:X:359:GLN:CD	1.48	1.35
2:X:183:SER:C	2:X:184:ALA:N	1.86	1.34
1:P:271:GLY:CA	3:P:1685:GNP:H8	1.58	1.32
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
1:P:304:GLN:CD	3:P:1685:GNP:H3'	1.60	1.23
1:P:268:VAL:O	3:P:1685:GNP:O3A	1.53	1.22
2:X:354:ASP:CB	2:X:357:THR:HG22	1.67	1.22
1:P:327:VAL:O	1:P:329:LYS:N	1.71	1.22
1:P:331:TYR:OH	1:P:536:GLU:O	1.54	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
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:HD2	2:X:106:LYS:N	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
2:X:352:ALA:CB	2:X:361:MET:HE2	1.79	1.12
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:183:SER:CA	2:X:184:ALA:N	2.13	1.10
2:X:354:ASP:HB2	2:X:359:GLN:NE2	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:302:ILE:HB	2:X:401:PHE:HB3	1.36	1.06
2:X:353:ILE:CG1	2:X:361:MET:H	1.68	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:352:ALA:C	2:X:361:MET:HG3	1.83	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
1:P:304:GLN:CD	3:P:1685:GNP:C3'	2.32	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:H	2:X:267:LEU:CD1	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:354:ASP:CB	2:X:359:GLN:CD	2.36	0.99
2:X:183:SER:C	2:X:184:ALA:CA	2.36	0.99
2:X:300:PHE:HD2	2:X:401:PHE:CZ	1.79	0.99
2:X:359:GLN:HG2	2:X:359:GLN:O	1.63	0.99
1:P:268:VAL:HG13	1:P:346:GLY:HA2	1.45	0.98
2:X:181:GLY:O	2:X:182:GLN:HG2	1.63	0.98
2:X:183:SER:CB	2:X:184:ALA:N	2.26	0.98
2:X:326:ILE:HG22	2:X:327:ARG:N	1.72	0.97
2:X:302:ILE:HG23	2:X:302:ILE:O	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:327:ARG:HH12	2:X:372:TRP:NE1	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:326:ILE:HG21	2:X:367:GLU:O	1.67	0.94
2:X:163:ARG:NH2	2:X:391:SER:HA	1.81	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: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:330:ALA:C	1:P:341:ILE:HG22	1.94	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
2:X:352:ALA:C	2:X:361:MET:CG	2.45	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:182:GLN:C	2:X:183:SER:CA	2.46	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:304:GLN:C	3:P:1685:GNP:HO3'	1.82	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:300:PHE:CD2	2:X:401:PHE:CZ	2.64	0.84
2:X:182:GLN:CB	2:X:183:SER:N	2.39	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:326:ILE:HG21	2:X:367:GLU:C	2.01	0.84
2:X:300:PHE:HD2	2:X:401:PHE:CE1	1.94	0.84
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
1:P:327:VAL:C	1:P:329:LYS:N	2.37	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:263:GLN:OE1	2:X:267:LEU:HD21	1.79	0.81
1:P:610:GLU:HG2	2:X:259:ASN:CG	2.06	0.81
2:X:106:LYS:H	2:X:106:LYS:HZ2	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: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:O	2:X:105:LYS:CG	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: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:352:ALA:HB2	2:X:361:MET:HE2	1.64	0.76
2:X:359:GLN:CG	2:X:359:GLN:O	2.32	0.76
1:P:405:ASN:OD1	3:P:1685:GNP:O6	2.03	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:105:LYS:C	2:X:106:LYS:HD2	2.09	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:273:SER:OG	1:P:325:ILE:HD12	1.86	0.75
1:P:348:LYS:HZ2	3:P:1685:GNP:PG	2.10	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:327:VAL:O	1:P:328:GLY:C	2.30	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:328:GLY:C	1:P:350:TYR:CZ	2.66	0.73
2:X:181:GLY:C	2:X:182:GLN:HG2	2.13	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:354:ASP:CG	2:X:357:THR:CG2	2.62	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:327:VAL:C	1:P:329:LYS:H	1.96	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:354:ASP:N	2:X:359:GLN:CD	2.47	0.72
2:X:375:ALA:O	2:X:376:ASN:ND2	2.23	0.71
2:X:327:ARG:HH12	2:X:372:TRP:CD1	2.07	0.71
1:P:304:GLN:CD	3:P:1685:GNP:O3'	2.33	0.71
2:X:263:GLN:O	2:X:267:LEU:HD13	1.89	0.71
2:X:333:ALA:C	2:X:335:ASP:H	1.99	0.71
2:X:354:ASP:HB2	2:X:359:GLN:CG	2.20	0.71
1:P:256:GLY:C	1:P:545:MET:HB3	2.15	0.71
2:X:352:ALA:HB3	2:X:361:MET:SD	2.30	0.71
2:X:348:ASP:C	2:X:350:SER:H	1.98	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: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:312:GLY:O	2:X:313:ALA:CB	2.40	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: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
2:X:342:ALA:C	2:X:346:ALA:HB3	2.18	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:268:VAL:O	3:P:1685:GNP:O1B	2.12	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
1:P:326:GLU:O	1:P:327:VAL:C	2.36	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:349:MET:HE2	2:X:255:TYR:HB2	1.77	0.67
1:P:392:ALA:HB1	1:P:397:VAL:HG11	1.76	0.67
2:X:104:GLU:C	2:X:104:GLU:CD	2.63	0.67
1:P:605:HIS:CE1	1:P:661:GLN:HE22	2.12	0.67
2:X:352:ALA:O	2:X:359:GLN:CD	2.38	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:N	2:X:106:LYS:HZ2	1.93	0.66
2:X:328:TYR:CD2	2:X:364:VAL:HB	2.30	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
2:X:267:LEU:CD1	2:X:267:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:299:CYS:C	2:X:406:ALA:H	2.06	0.63
2:X:161:ASN:CG	2:X:390:LYS:HB2	2.17	0.62
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
1:P:271:GLY:C	3:P:1685:GNP:O1A	2.42	0.62
2:X:12:TRP:CE3	2:X:321:GLU:CD	2.77	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: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
2:X:390:LYS:O	2:X:391:SER:HB3	1.98	0.62
1:P:288:LYS:HB2	1:P:291:ILE:HG22	1.82	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
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:183:SER:C	2:X:184:ALA:HA	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:333:ALA:C	2:X:335:ASP:N	2.59	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:CD	2:X:106:LYS:H	2.11	0.59
2:X:163:ARG:HH12	2:X:391:SER:CB	2.15	0.59
2:X:24:ALA:HB3	2:X:31:MET:HE3	1.85	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:257:LYS:HE2	1:P:546:CYS:SG	2.43	0.58
1:P:259:HIS:CD2	1:P:338:ARG:H	2.22	0.58
2:X:223:LEU:HD11	2:X:233:LEU:HD12	1.86	0.58
2:X:300:PHE:CE2	2:X:401:PHE:CE1	2.90	0.58
2:X:354:ASP:O	2:X:357:THR:HG22	2.02	0.58
2:X:161:ASN:HD22	2:X:390:LYS:HB2	0.78	0.58
1:P:405:ASN:CG	3:P:1685:GNP:O6	2.47	0.58
1:P:591:LYS:HE3	1:P:591:LYS:HA	1.86	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	2:X:409:ARG:NH1	2.63	0.57
2:X:314:VAL:CG1	2:X:406:ALA:HB1	2.35	0.56
1:P:259:HIS:CE1	1:P:545:MET:HE1	2.39	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
1:P:312:MET:HE3	1:P:312:MET:HA	1.88	0.56
2:X:101:ASP:O	2:X:102:GLY:C	2.48	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: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
2:X:354:ASP:CA	2:X:359:GLN:CD	2.80	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:304:GLN:C	3:P:1685:GNP:O3'	2.41	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
1:P:331:TYR:CE1	1:P:536:GLU:CD	2.86	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:105:LYS:O	2:X:106:LYS:C	2.51	0.54
2:X:330:PHE:O	2:X:330:PHE:CG	2.61	0.54
1:P:265:MET:CG	1:P:354:MET:HE1	2.38	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:263:GLN:C	2:X:267:LEU:HD21	2.32	0.54
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: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
2:X:311:LEU:O	2:X:312:GLY:C	2.52	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:605:HIS:CE1	1:P:661:GLN:CD	2.87	0.53
1:P:329:LYS:HE3	1:P:329:LYS:HA	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
2:X:182:GLN:C	2:X:183:SER:HA	2.34	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:678:LYS:HZ2	1:P:680:VAL:HA	1.74	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:365:VAL:HA	1:P:400:MET:O	2.09	0.52
1:P:366:LEU:HD11	1:P:385:THR:HG23	1.90	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:263:GLN:CD	2:X:267:LEU:HD21	2.35	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:342:ALA:HA	2:X:346:ALA:HB1	1.89	0.51
2:X:386:PHE:C	2:X:387:ILE:HG13	2.35	0.51
1:P:356:GLY:HA3	1:P:605:HIS:CG	2.45	0.51
1:P:263:ILE:HG12	1:P:354:MET:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:575:ILE:CG1	1:P:659:TYR:CE1	2.94	0.51
2:X:9:ILE:CG2	2:X:374:ALA:CB	2.87	0.51
2:X:30:SER:HB3	2:X:67:SER:HB3	1.93	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
2:X:253:VAL:HG21	2:X:260:GLY:C	2.35	0.51
2:X:275:VAL:C	2:X:276:LYS:HG3	2.36	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
2:X:354:ASP:CG	2:X:357:THR:HG22	2.27	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
2:X:348:ASP:C	2:X:350:SER:N	2.65	0.50
1:P:269:ASP:O	3:P:1685:GNP:O4'	2.29	0.50
2:X:9:ILE:HD12	2:X:371:GLU:HA	1.94	0.50
2:X:12:TRP:CD2	2:X:321:GLU:HB2	2.46	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
2:X:352:ALA:C	2:X:361:MET:HG2	2.36	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:5:VAL:HG23	2:X:385:GLU:HB3	1.94	0.50
2:X:145:PHE:CE1	2:X:158:VAL:HG12	2.46	0.50
1:P:324:THR:HG23	1:P:348:LYS:CD	2.42	0.50
1:P:330:ALA:CA	1:P:341:ILE:HG22	2.41	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

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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	0.49
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:35:VAL:HG22	2:X:91:VAL:HG13	1.94	0.49
2:X:263:GLN:C	2:X:267:LEU:CD2	2.86	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
1:P:316:LYS:CG	1:P:325:ILE:HG12	2.39	0.49
1:P:319:ARG:NH1	1:P:327:VAL:HA	2.28	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
1:P:256:GLY:H	1:P:545:MET:HE2	1.78	0.49
2:X:125:ASP:CG	2:X:126:ASN:H	2.20	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:4:GLU:HG2	2:X:283:LEU:HD22	1.94	0.49
2:X:291:ILE:O	2:X:291:ILE:HG22	2.13	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:259:HIS:CG	1:P:545:MET:CE	2.96	0.49
1:P:268:VAL:HA	3:P:1685:GNP:O1B	2.13	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:256:GLY:O	1:P:545:MET:HB3	2.14	0.48
1:P:345:PRO:HA	1:P:348:LYS:CG	2.43	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:536:GLU:HB3	1:P:548:GLU:CD	2.37	0.48
1:P:575:ILE:HG12	1:P:659:TYR:CZ	2.49	0.48
2:X:53:TYR:CE1	2:X:69:LEU:HG	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
1:P:256:GLY:N	1:P:545:MET:HE2	2.27	0.48
1:P:257:LYS:HD3	1:P:258:ASP:H	1.78	0.48
1:P:409:ASP:HB3	3:P:1685:GNP:HN21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:298:ALA:C	1:P:299:LYS:HG3	2.38	0.48
2:X:9:ILE:HD12	2:X:370:ILE:HG22	1.96	0.48
2:X:338:VAL:O	2:X:339:ILE:HD13	2.14	0.48
1:P:257:LYS:HD2	1:P:258:ASP:H	1.77	0.48
1:P:262:LEU:HD23	1:P:262:LEU:C	2.39	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
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:HG2	1:P:316:LYS:O	2.14	0.48
1:P:619:LYS:HG2	1:P:620:LEU:HD12	1.96	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:354:ASP:CG	2:X:357:THR:HG21	2.33	0.47
2:X:186:ARG:O	2:X:186:ARG:HG2	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:362:ASP:O	2:X:363:VAL:C	2.55	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:257:LYS:HA	1:P:545:MET:SD	2.54	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
2:X:327:ARG:HG2	2:X:369:LEU:HG	1.96	0.47
1:P:259:HIS:HB3	1:P:338:ARG:HB2	1.97	0.47
1:P:385:THR:HG21	1:P:429:PHE:CE2	2.49	0.47
1:P:391:LEU:HD23	1:P:603:HIS:HD1	1.79	0.47
1:P:406:LYS:NZ	3:P:1685:GNP:N3	2.56	0.47
1:P:596:ALA:HB1	1:P:615:LYS:HA	1.97	0.47
2:X:101:ASP:C	2:X:103:LYS:N	2.73	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:317:GLU:O	1:P:321:ASP:OD1	2.33	0.47
1:P:458:VAL:C	1:P:460:PRO:HD3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:659:TYR:CD1	1:P:659:TYR:N	2.83	0.47
1:P:328:GLY:C	1:P:350:TYR:OH	2.58	0.46
1:P:354:MET:HE3	1:P:392:ALA:HB2	1.97	0.46
2:X:327:ARG:CZ	2:X:372:TRP:CD1	2.98	0.46
2:X:104:GLU:CD	2:X:105:LYS:N	2.73	0.46
1:P:255:GLY:O	1:P:544:ALA:HA	2.15	0.46
1:P:444:MET:HE3	1:P:445:PRO:O	2.15	0.46
2:X:9:ILE:O	2:X:9:ILE:HG12	2.16	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
1:P:366:LEU:HD13	1:P:366:LEU:HA	1.73	0.46
2:X:358:GLY:O	2:X:360:GLU:N	2.47	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:348:LYS:HZ3	3:P:1685:GNP:PG	2.37	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:342:LEU:C	1:P:342:LEU:HD23	2.40	0.46
1:P:577:SER:HB2	1:P:652:CYS:HA	1.97	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
2:X:258:GLU:CD	2:X:258:GLU:H	2.24	0.46
2:X:302:ILE:HG12	2:X:401:PHE:HB3	1.96	0.46
2:X:330:PHE:CD1	2:X:330:PHE:O	2.69	0.46
2:X:338:VAL:C	2:X:339:ILE:HD13	2.41	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
2:X:326:ILE:HG23	2:X:368:PRO:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:578:VAL:HG12	1:P:579:THR:N	2.31	0.45
2:X:7:LYS:HE3	2:X:277:TYR:CE1	2.51	0.45
2:X:147:VAL:CG2	2:X:261:PHE:CZ	2.99	0.45
2:X:331:LYS:CE	2:X:361:MET:SD	3.04	0.45
1:P:309:SER:HB2	1:P:448:GLY:C	2.41	0.45
1:P:343:ASP:OD2	1:P:350:TYR:HE2	2.00	0.45
1:P:616:LEU:C	1:P:616:LEU:HD23	2.42	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: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: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:268:VAL:C	3:P:1685:GNP:O1B	2.59	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:38:PRO:HA	2:X:85:LEU:CD1	2.47	0.45
2:X:299:CYS:O	2:X:406:ALA:N	2.50	0.45
2:X:354:ASP:O	2:X:357:THR:N	2.49	0.45
2:X:353:ILE:CG1	2:X:361:MET:HB2	2.36	0.45
1:P:549:GLN:HG2	1:P:550:VAL:N	2.31	0.45
1:P:540:GLU:O	1:P:541:VAL:HG22	2.16	0.44
1:P:298:ALA:HB3	1:P:299:LYS:HZ3	1.81	0.44
1:P:496:LYS:HZ3	1:P:502:THR:HG21	1.81	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:301:GLY:HA2	2:X:404:ILE:H	1.83	0.44
2:X:317:LEU:HD21	2:X:373:LEU:HD13	1.99	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:183:SER:C	2:X:184:ALA:C	2.85	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
1:P:331:TYR:OH	1:P:536:GLU:CG	2.47	0.44
1:P:333:GLU:HB2	1:P:338:ARG:CG	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:9:ILE:HD11	2:X:371:GLU:HG2	2.00	0.44
2:X:357:THR:CG2	2:X:359:GLN:H	2.28	0.44
1:P:283:THR:HG21	1:P:333:GLU:HB3	1.98	0.44
2:X:354:ASP:CB	2:X:359:GLN:CG	2.91	0.44
2:X:6:GLU:HG2	2:X:384:LEU:O	2.18	0.43
2:X:300:PHE:O	2:X:300:PHE:CG	2.70	0.43
2:X:343:GLU:H	2:X:346:ALA:CB	2.31	0.43
1:P:308:LEU:HA	1:P:310:TRP:CD2	2.54	0.43
1:P:463:CYS:SG	1:P:464:PRO:HD3	2.58	0.43
2:X:319:VAL:O	2:X:386:PHE:CA	2.65	0.43
1:P:259:HIS:CG	1:P:545:MET:HE1	2.53	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:258:ASP:C	1:P:259:HIS:HD1	2.27	0.43
1:P:259:HIS:ND1	1:P:545:MET:HE1	2.33	0.43
1:P:351:VAL:HG21	1:P:388:HIS:CG	2.53	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: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:O	1:P:547:GLY:HA3	2.18	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
1:P:440:ASP:O	1:P:441:VAL:HG13	2.19	0.43
2:X:6:GLU:HA	2:X:385:GLU:HA	1.99	0.43
2:X:176:LYS:C	2:X:178:GLY:H	2.27	0.43
2:X:264:ALA:HA	2:X:267:LEU:HD22	2.01	0.43
2:X:351:PHE:C	2:X:353:ILE:H	2.26	0.43
2:X:375:ALA:C	2:X:376:ASN:CG	2.86	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:597:GLY:C	2:X:396:GLN:HE21	2.25	0.43
2:X:358:GLY:O	2:X:359:GLN:C	2.61	0.43
2:X:389:ASP:HB2	2:X:394:GLY:C	2.44	0.43
1:P:255:GLY:N	1:P:548:GLU:CD	2.77	0.43
1:P:297:GLU:CD	1:P:298:ALA:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:347:LYS:C	2:X:363:VAL:HG21	2.43	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
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
2:X:407:MET:HB3	2:X:407:MET:HE3	1.82	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:181:GLY:C	2:X:182:GLN:CG	2.85	0.42
2:X:43:PRO:HA	2:X:46:GLN: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
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: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:326:GLU:HB2	1:P:343:ASP:CG	2.44	0.42
1:P:299:LYS:CD	1:P:310:TRP:HB2	2.49	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
2:X:9:ILE:HG21	2:X:374:ALA:HB3	2.00	0.42
2:X:160:GLY:HA2	2:X:278:VAL:HB	2.01	0.42
2:X:352:ALA:O	2:X:361:MET:CG	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:581:PHE:CZ	1:P:602:MET:HE1	2.54	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:9:ILE:HB	2:X:386:PHE:CE1	2.55	0.41
2:X:30:SER:HB2	2:X:71:ALA:HB2	2.01	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:263:ILE:HD12	1:P:361:ALA:HB2	2.01	0.41
1:P:264:PHE:HE1	1:P:341:ILE:HD11	1.85	0.41
1:P:268:VAL:HG22	1:P:347:HIS:H	1.85	0.41
1:P:345:PRO:HB2	1:P:384:GLN:OE1	2.20	0.41
1:P:507:LYS:HE2	1:P:547:GLY:HA2	2.01	0.41
1:P:522:MET:HE3	1:P:522:MET:HA	2.02	0.41
1:P:610:GLU:CB	2:X:259:ASN:OD1	2.65	0.41
2:X:155:PHE:CZ	2:X:205:VAL:HG23	2.56	0.41
2:X:386:PHE:O	2:X:387:ILE:HG13	2.20	0.41
2:X:400:GLY:C	2:X:401:PHE:CD1	2.98	0.41
2:X:284:LEU:CD2	2:X:387:ILE:HD11	2.50	0.41
2:X:287:TYR:CB	2:X:318:ILE:HD11	2.44	0.41
1:P:277:GLY:N	1:P:326:GLU:OE2	2.54	0.41
1:P:304:GLN:OE1	3:P:1685:GNP:H5'1	2.21	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:121:LEU:HD13	2:X:129:HIS:C	2.46	0.41
2:X:317:LEU:O	2:X:385:GLU:N	2.52	0.41
2:X:319:VAL:HG21	2:X:373:LEU:CD1	2.51	0.41
1:P:258:ASP:OD1	1:P:481:VAL:N	2.54	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
2:X:352:ALA:HB1	2:X:361:MET:SD	2.61	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
1:P:321:ASP:C	1:P:323:LYS:H	2.23	0.41
2:X:211:ILE:HA	2:X:216:VAL:HA	2.02	0.41
2:X:240:ASP:O	2:X:241:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:283:LEU:O	2:X:287:TYR:CD2	2.73	0.41
1:P:355:ILE:CD1	1:P:392:ALA:H	2.32	0.41
1:P:356:GLY:CA	1:P:605:HIS:CD2	3.04	0.41
1:P:500:LEU:HD13	1:P:500:LEU:C	2.46	0.41
2:X:330:PHE:CD1	2:X:330:PHE:C	2.98	0.41
1:P:279:LEU:O	1:P:332:PHE:CD2	2.74	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:308:LEU:C	1:P:310:TRP:H	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:258:ASP:CG	1:P:480:HIS:HB2	2.46	0.40
1:P:330:ALA:CB	1:P:341:ILE:HG22	2.51	0.40
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: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
2:X:351:PHE:C	2:X:353:ILE:N	2.80	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	3
2	X	420/437 (96%)	297 (71%)	58 (14%)	65 (16%)	0	3
All	All	848/867 (98%)	596 (70%)	127 (15%)	125 (15%)	0	3

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	299 (82%)	66 (18%)	2	9
2	X	362/377 (96%)	284 (78%)	78 (22%)	1	6
All	All	727/742 (98%)	583 (80%)	144 (20%)	3	7

All (144) 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	323	LYS
1	P	329	LYS
1	P	332	PHE
1	P	340	THR
1	P	341	ILE
1	P	342	LEU
1	P	343	ASP
1	P	350	TYR
1	P	355	ILE
1	P	366	LEU
1	P	374	GLU
1	P	375	TYR
1	P	377	THR
1	P	381	ARG

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Mol	Chain	Res	Type
1	P	384	GLN
1	P	386	ARG
1	P	394	THR
1	P	395	GLN
1	P	400	MET
1	P	403	VAL
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
1	P	461	LYS
1	P	482	ASP
1	P	485	ILE
1	P	522	MET
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	575	ILE
1	P	576	LYS
1	P	577	SER
1	P	579	THR
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	655	THR
1	P	678	LYS
1	P	681	LYS
2	X	13	LYS
2	X	25	ARG
2	X	41	LEU

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Mol	Chain	Res	Type
2	X	42	ILE
2	X	43	PRO
2	X	50	THR
2	X	52	GLU
2	X	58	ASN
2	X	65	ARG
2	X	78	LYS
2	X	79	LEU
2	X	85	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
2	X	118	ASN
2	X	119	THR
2	X	133	LEU
2	X	136	LEU
2	X	137	LEU
2	X	140	ASP
2	X	141	ASP
2	X	143	PHE
2	X	158	VAL
2	X	163	ARG
2	X	166	LEU
2	X	168	LYS
2	X	187	PHE
2	X	208	GLN
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	258	GLU
2	X	263	GLN

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Mol	Chain	Res	Type
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	330	PHE
2	X	331	LYS
2	X	334	GLU
2	X	337	GLU
2	X	340	LYS
2	X	355	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	320	ASN
1	P	486	ASN
1	P	539	ASN
1	P	573	ASN
1	P	605	HIS

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Mol	Chain	Res	Type
2	X	76	GLN
2	X	161	ASN
2	X	177	HIS
2	X	196	HIS
2	X	208	GLN
2	X	274	ASN
2	X	279	GLN
2	X	376	ASN
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 oligosaccharides 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	-	34,34,34	1.62	5 (14%)	47,54,54	1.12	4 (8%)

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	-	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1685	GNP	PA-O3A	-5.40	1.53	1.59
3	P	1685	GNP	PB-O3A	-4.43	1.53	1.59
3	P	1685	GNP	PB-O2B	-3.21	1.48	1.56
3	P	1685	GNP	PG-O2G	-3.18	1.48	1.56
3	P	1685	GNP	PG-O1G	2.31	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1685	GNP	O2B-PB-O1B	3.46	117.29	109.87
3	P	1685	GNP	O2G-PG-O3G	3.40	116.73	107.59
3	P	1685	GNP	O3G-PG-O1G	-3.15	105.56	113.45
3	P	1685	GNP	O1G-PG-N3B	-2.64	107.89	111.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	1685	GNP	PB-N3B-PG-O1G
3	P	1685	GNP	PG-N3B-PB-O1B
3	P	1685	GNP	PG-N3B-PB-O3A
3	P	1685	GNP	PA-O3A-PB-O1B

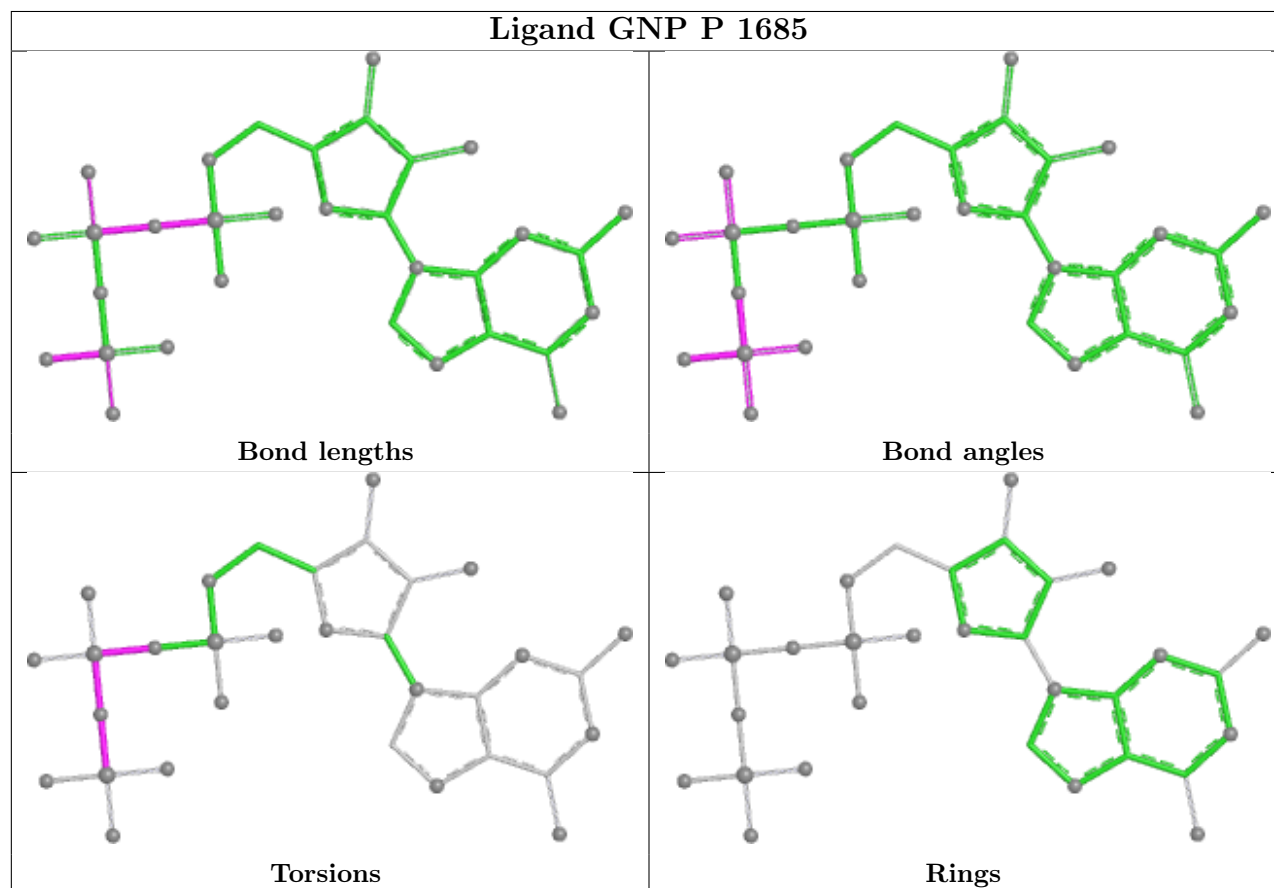
There are no ring outliers.

1 monomer is involved in 56 short contacts:

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

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	X	4
1	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	183:SER	C	184:ALA	N	1.86
1	X	182:GLN	C	183:SER	N	1.71
1	P	330:ALA	C	331:TYR	N	1.66
1	X	269:ALA	C	270:GLU	N	1.10
1	X	421:SER	C	422:GLU	N	1.00

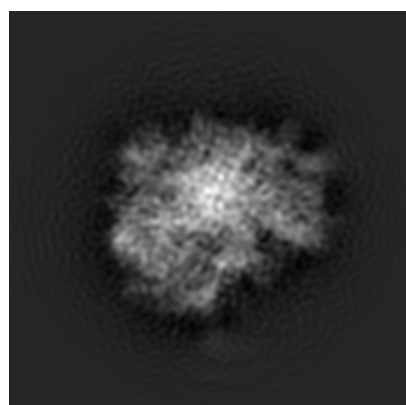
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2597. These allow visual inspection of the internal detail of the map and identification of artifacts.

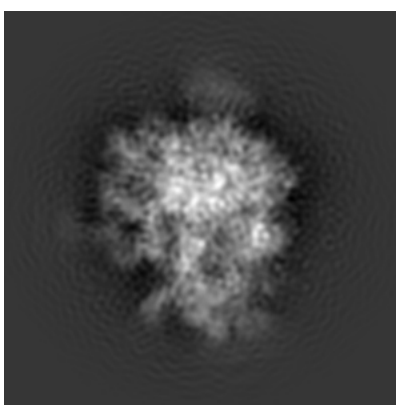
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

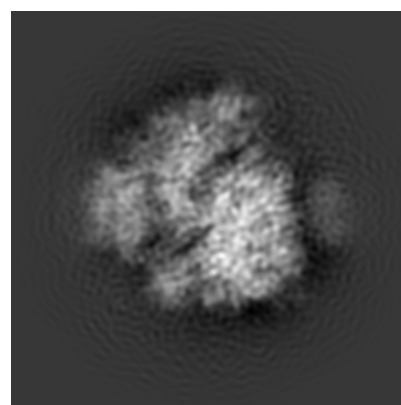
6.1.1 Primary map



X



Y

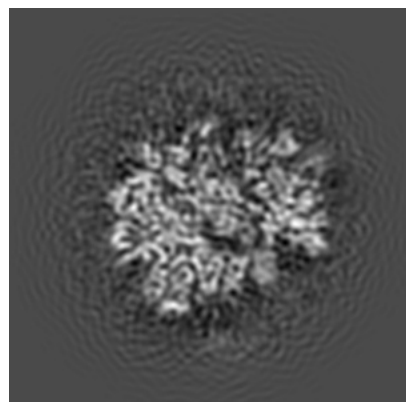


Z

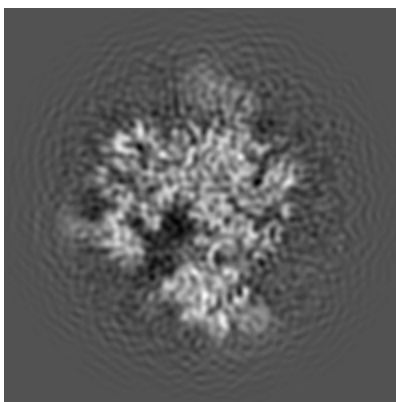
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

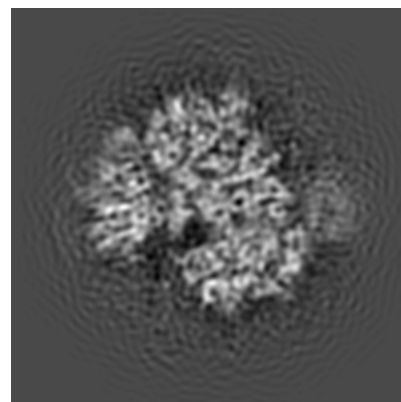
6.2.1 Primary map



X Index: 184



Y Index: 184

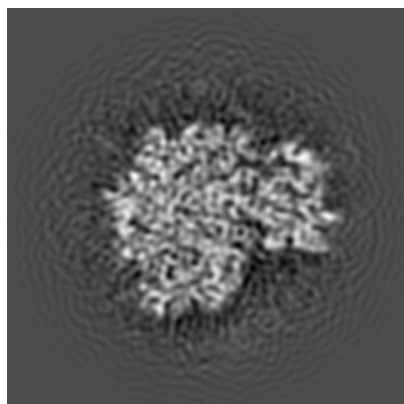


Z Index: 184

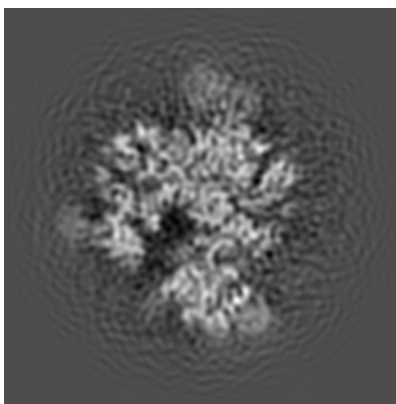
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

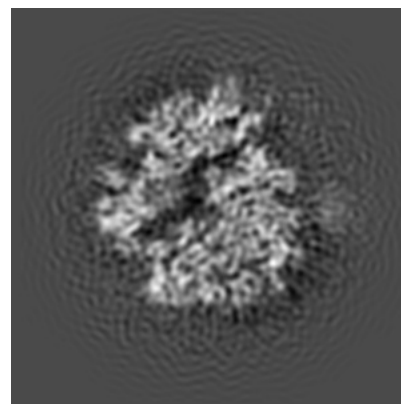
6.3.1 Primary map



X Index: 194



Y Index: 186

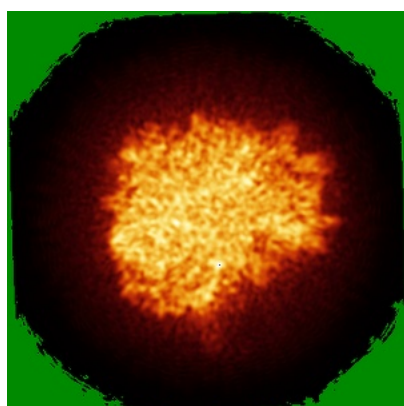


Z Index: 168

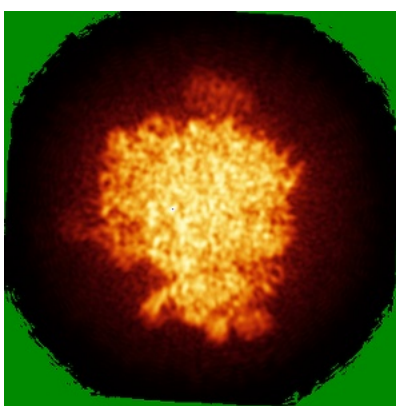
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

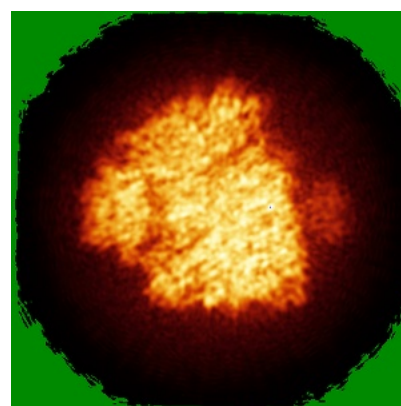
6.4.1 Primary map



X



Y

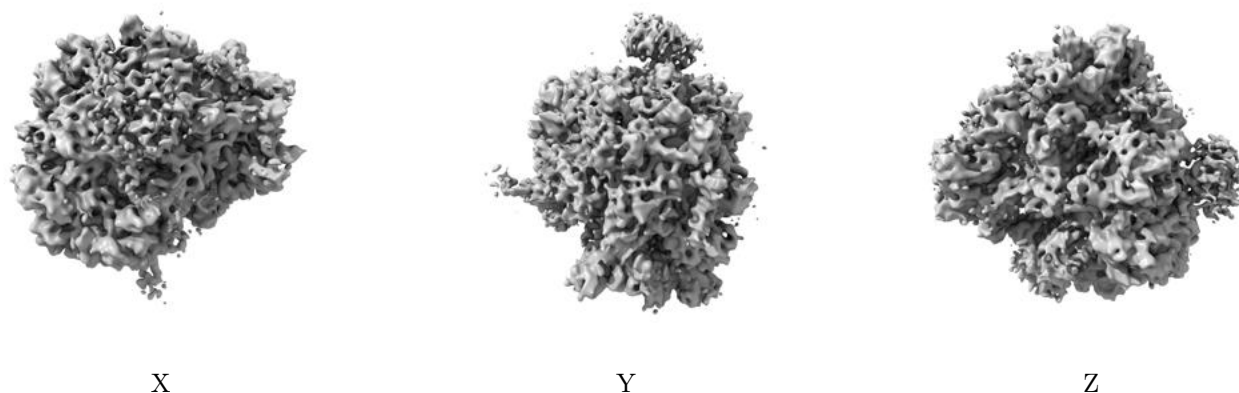


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.183. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

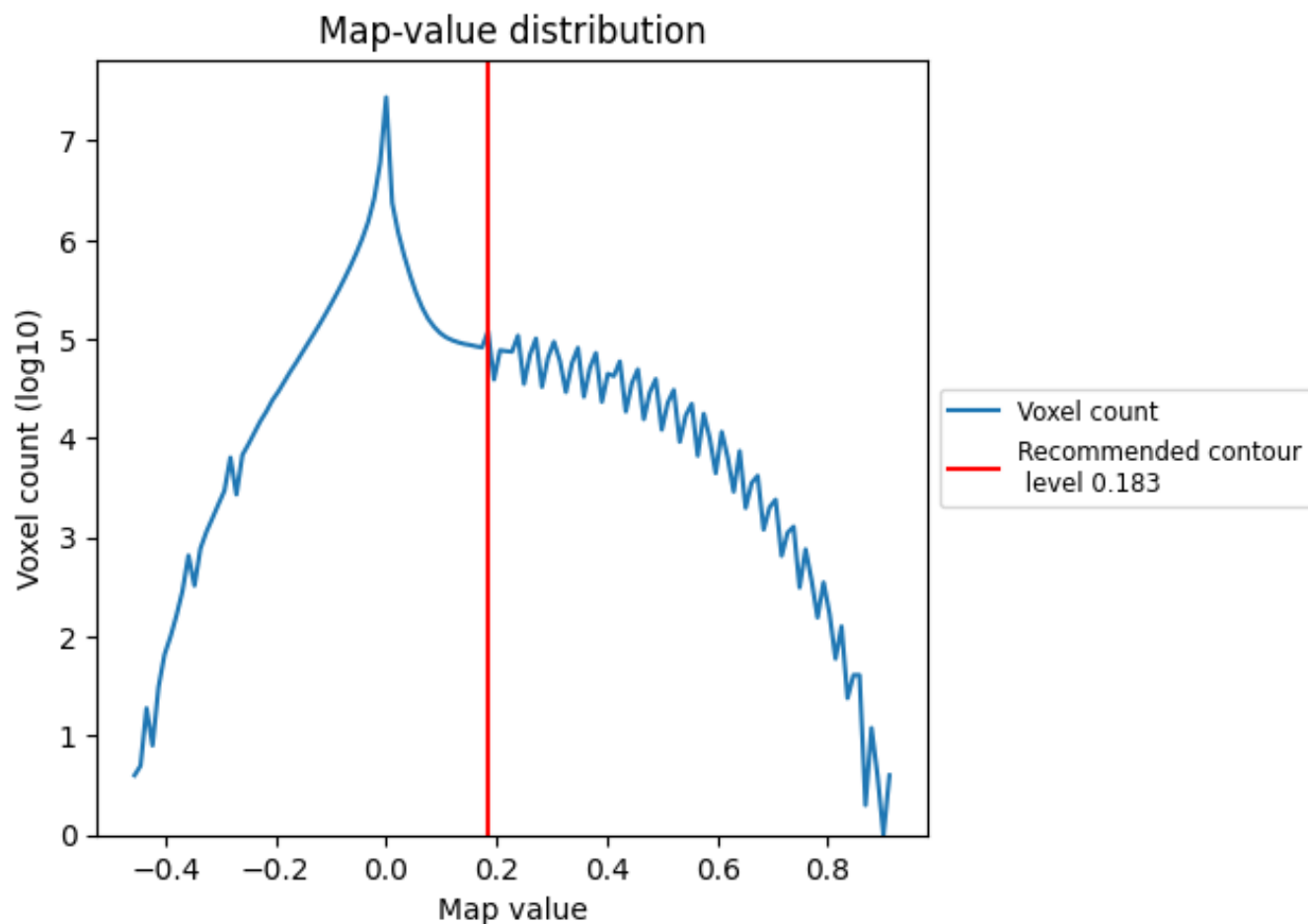
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

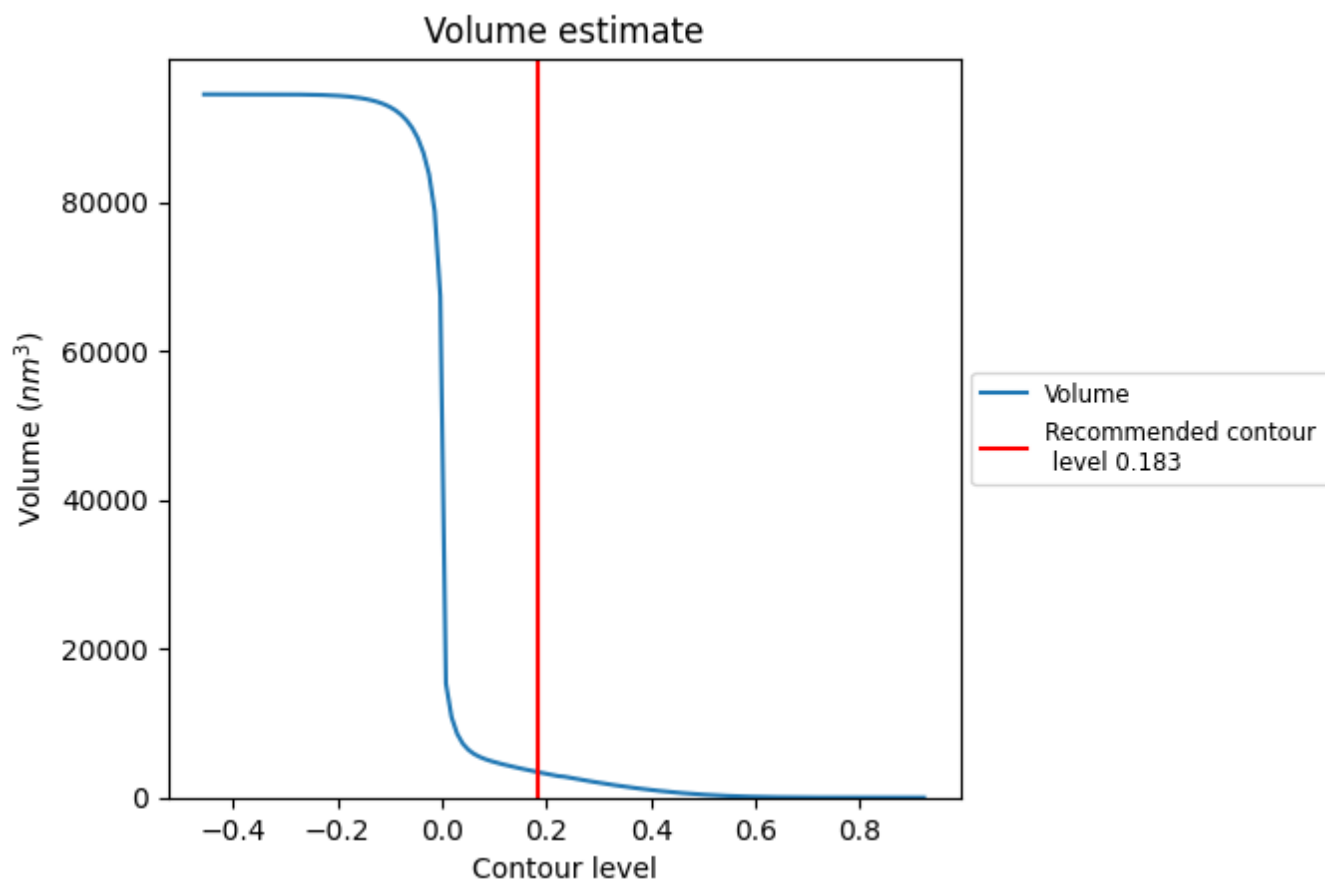
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

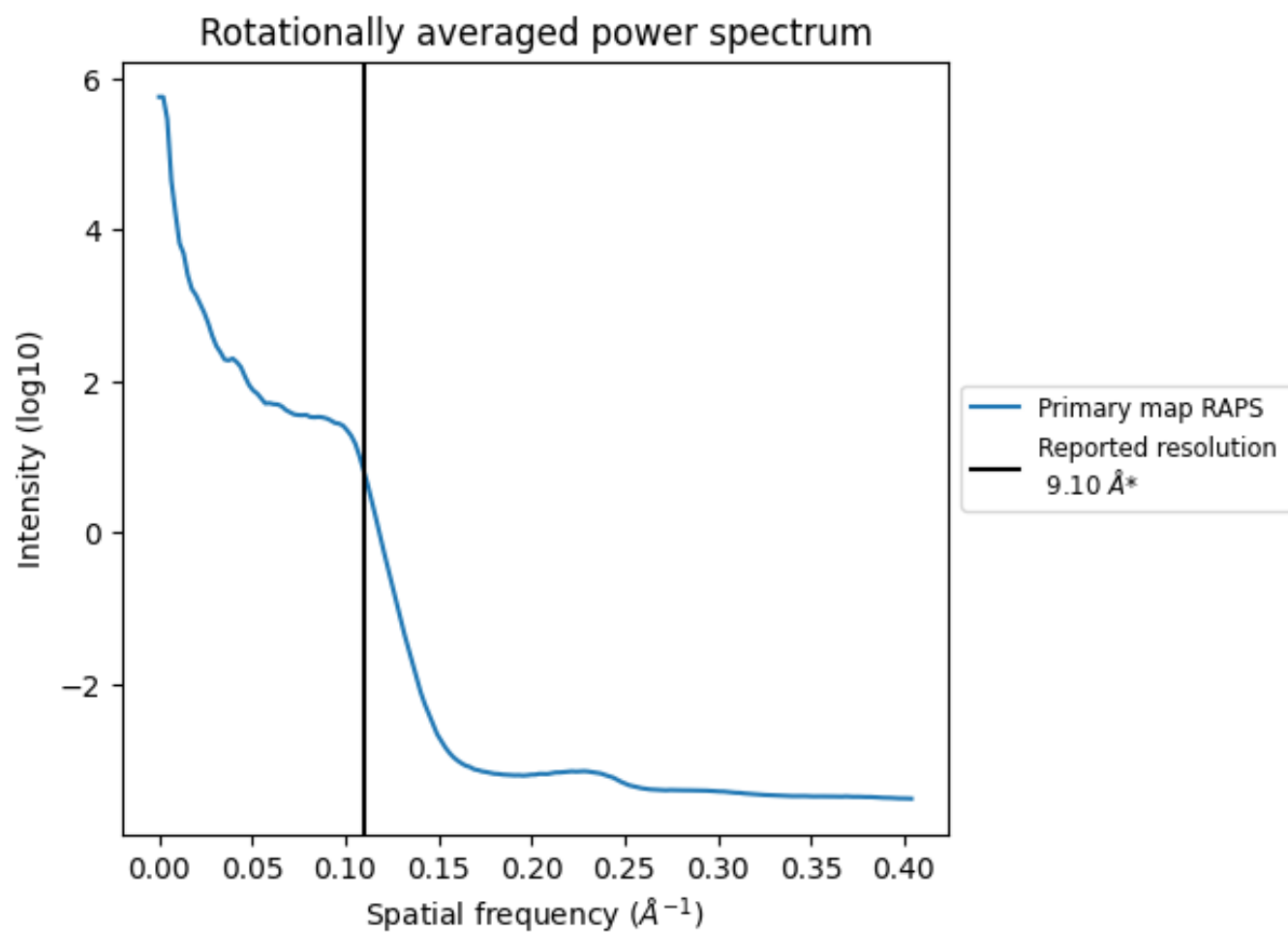
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3424 nm³; this corresponds to an approximate mass of 3093 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.110 Å⁻¹

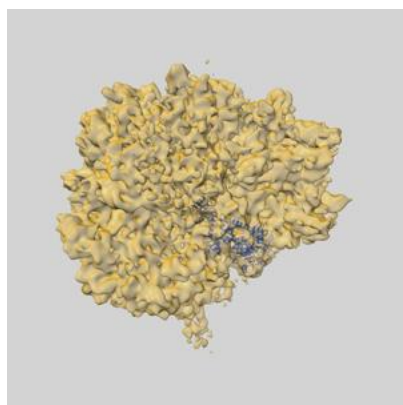
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

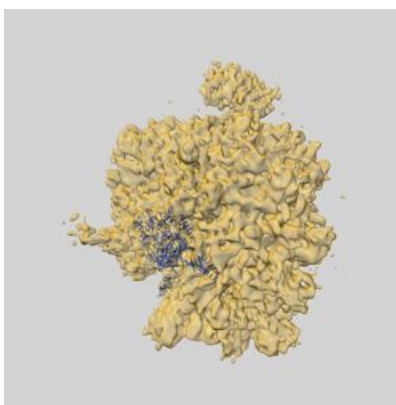
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2597 and PDB model 4CRN. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

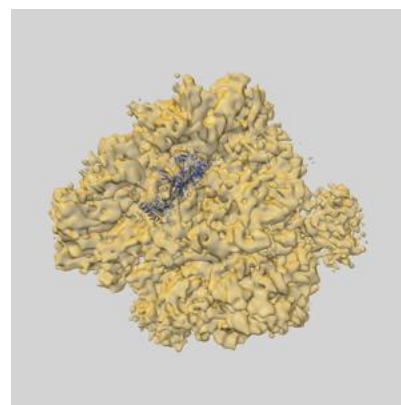
9.1 Map-model overlay [i](#)



X



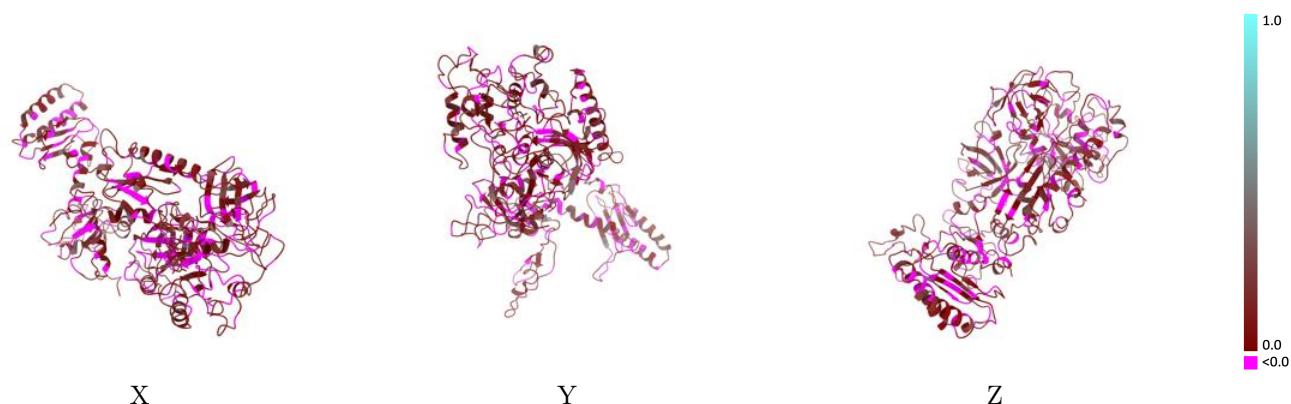
Y



Z

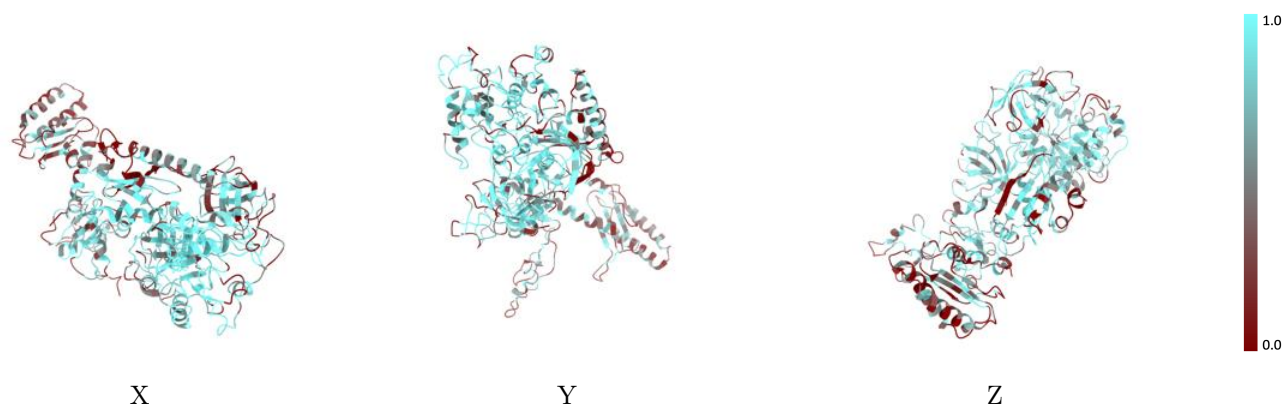
The images above show the 3D surface view of the map at the recommended contour level 0.183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



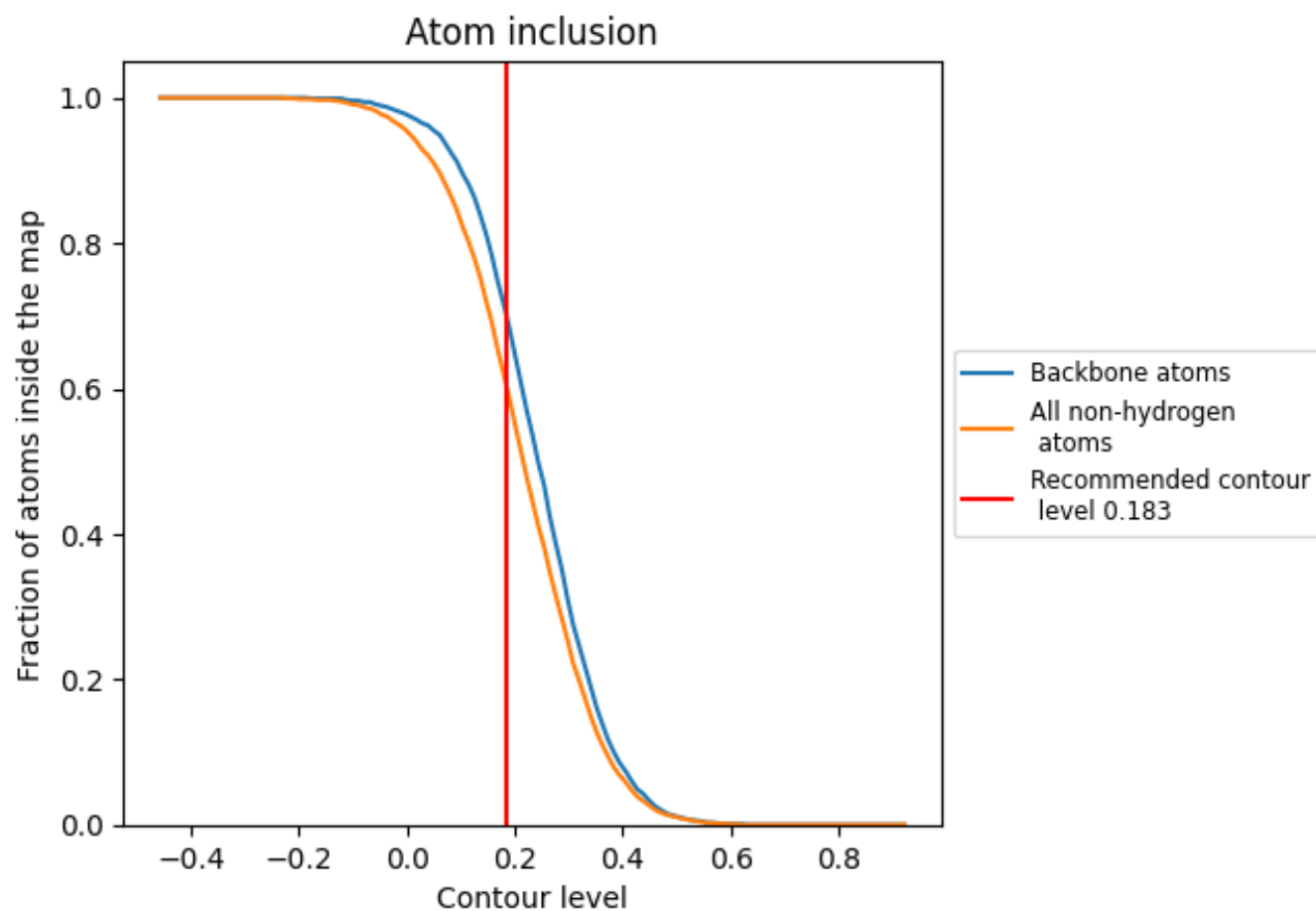
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.183).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6100	0.0750
P	0.7140	0.0740
X	0.5040	0.0750

