Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:23 AM GMT

PDB ID	:	2AAT
Title	:	2.8-ANGSTROMS-RESOLUTION CRYSTAL STRUCTURE OF AN ACTIVE-SITE MUTANT OF ASPARTATE AMINOTRANSFERASE FROM ESCHERICHIA COLI
Authors	:	Smith, D.; Almo, S.; Toney, M.; Ringe, D.
Deposited on	:	1989-05-30
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

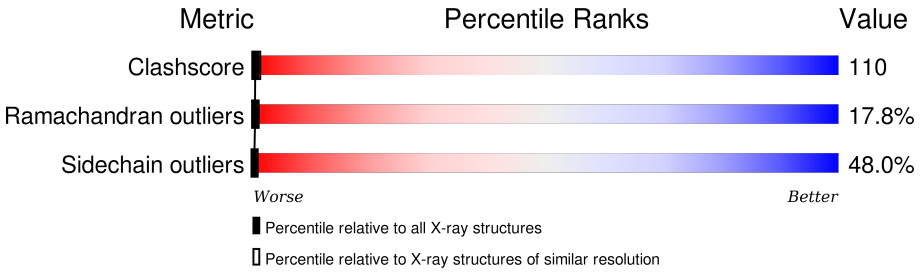
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	7% 29% 35% 30%

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	PMP	A	1	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3086 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

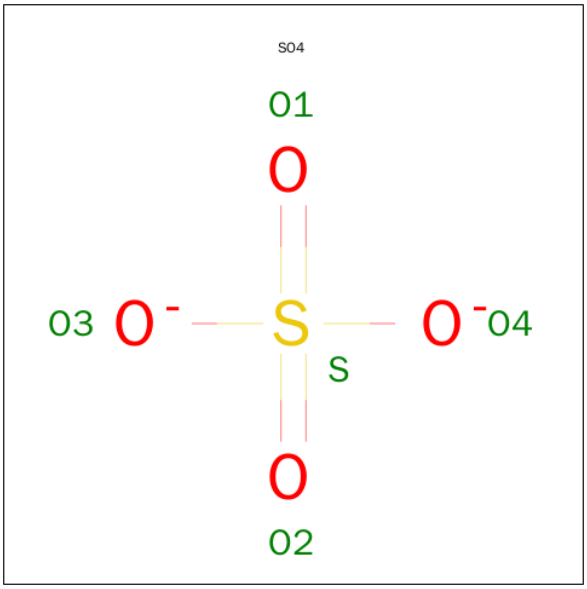
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3065	1933	535	584	13			

There is a discrepancy between the modelled and reference sequences:

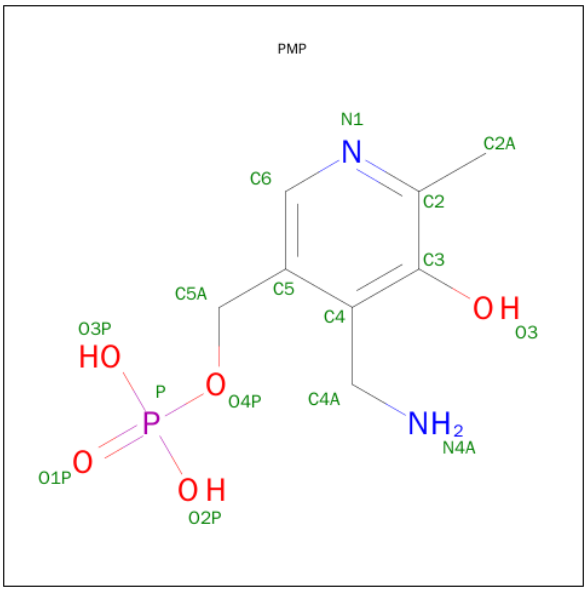
Chain	Residue	Modelled	Actual	Comment	Reference
A	258	ALA	LYS	ENGINEERED MUTATION	UNP P00509

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	16	8	2	5	1	0	0

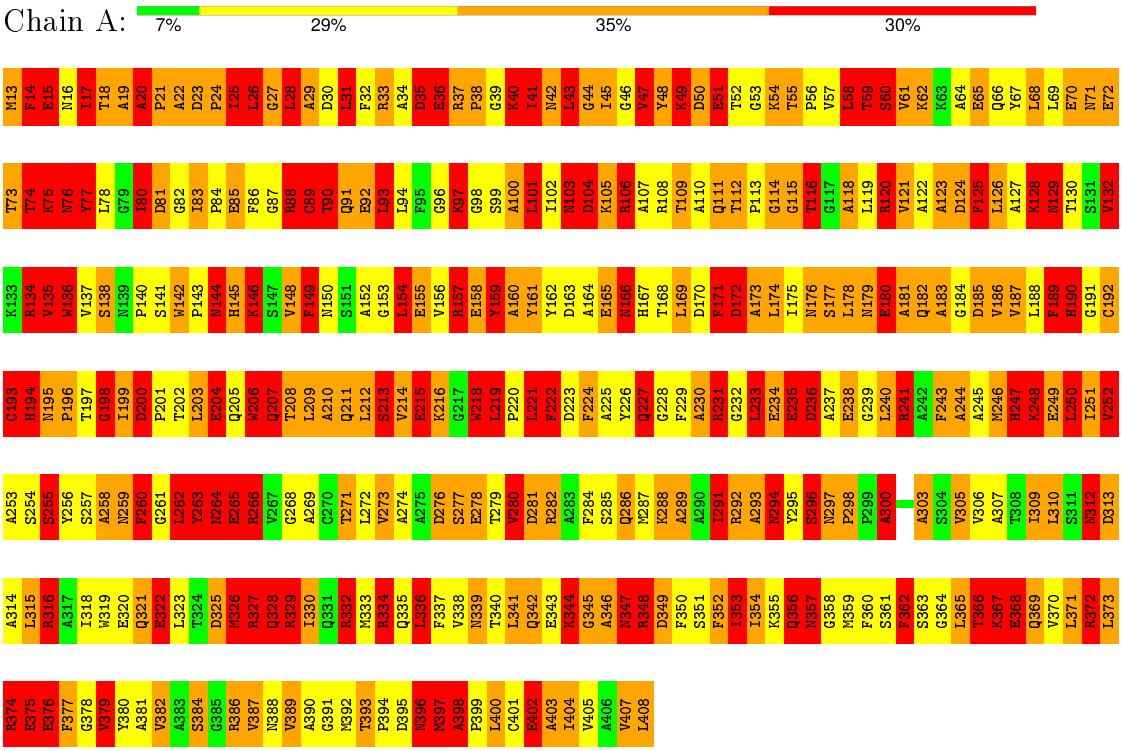
3 Residue-property plots (i)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	156.80Å 86.74Å 79.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3086	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PMP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.94	26/3126 (0.8%)	3.03	330/4236 (7.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	GLU	CD-OE2	8.22	1.34	1.25
1	A	278	GLU	CD-OE2	7.32	1.33	1.25
1	A	36	GLU	CD-OE2	6.76	1.33	1.25
1	A	51	GLU	CD-OE2	6.57	1.32	1.25
1	A	215	GLU	CD-OE2	6.40	1.32	1.25
1	A	235	GLU	CD-OE2	6.37	1.32	1.25
1	A	155	GLU	CD-OE2	6.31	1.32	1.25
1	A	265	GLU	CD-OE2	6.13	1.32	1.25
1	A	180	GLU	CD-OE2	6.04	1.32	1.25
1	A	158	GLU	CD-OE2	5.99	1.32	1.25
1	A	204	GLU	CD-OE2	5.94	1.32	1.25
1	A	368	GLU	CD-OE2	5.91	1.32	1.25
1	A	320	GLU	CD-OE2	5.90	1.32	1.25
1	A	249	GLU	CD-OE2	5.89	1.32	1.25
1	A	343	GLU	CD-OE2	5.87	1.32	1.25
1	A	85	GLU	CD-OE2	5.79	1.32	1.25
1	A	70	GLU	CD-OE2	5.79	1.32	1.25
1	A	15	GLU	CD-OE2	5.75	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	GLU	CD-OE2	5.74	1.31	1.25
1	A	92	GLU	CD-OE2	5.69	1.31	1.25
1	A	72	GLU	CD-OE2	5.67	1.31	1.25
1	A	238	GLU	CD-OE2	5.66	1.31	1.25
1	A	165	GLU	CD-OE2	5.44	1.31	1.25
1	A	65	GLU	CD-OE2	5.41	1.31	1.25
1	A	376	GLU	CD-OE2	5.37	1.31	1.25
1	A	375	GLU	CD-OE2	5.25	1.31	1.25

All (330) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	ARG	CD-NE-CZ	40.20	179.89	123.60
1	A	372	ARG	CD-NE-CZ	24.55	157.97	123.60
1	A	292	ARG	NE-CZ-NH2	18.02	129.31	120.30
1	A	362	PHE	CA-CB-CG	16.89	154.44	113.90
1	A	379	VAL	CB-CA-C	16.76	143.25	111.40
1	A	334	ARG	NE-CZ-NH1	16.52	128.56	120.30
1	A	213	SER	N-CA-CB	14.63	132.45	110.50
1	A	193	CYS	C-N-CA	14.37	157.63	121.70
1	A	328	GLN	CB-CG-CD	13.02	145.45	111.60
1	A	231	ARG	NE-CZ-NH1	-12.80	113.90	120.30
1	A	155	GLU	N-CA-CB	12.78	133.60	110.60
1	A	23	ASP	CB-CG-OD1	12.72	129.75	118.30
1	A	21	PRO	N-CA-C	12.61	144.89	112.10
1	A	88	ARG	NE-CZ-NH1	12.51	126.56	120.30
1	A	211	GLN	CA-CB-CG	12.45	140.80	113.40
1	A	161	TYR	CB-CG-CD2	-12.44	113.53	121.00
1	A	334	ARG	CD-NE-CZ	12.25	140.75	123.60
1	A	386	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	A	348	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	A	374	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	A	211	GLN	N-CA-CB	12.09	132.35	110.60
1	A	136	TRP	N-CA-CB	12.08	132.34	110.60
1	A	172	ASP	CB-CG-OD2	-12.02	107.49	118.30
1	A	366	THR	N-CA-CB	11.88	132.87	110.30
1	A	349	ASP	CB-CG-OD1	11.88	128.99	118.30
1	A	161	TYR	CB-CG-CD1	11.87	128.12	121.00
1	A	349	ASP	CA-CB-CG	11.73	139.20	113.40
1	A	231	ARG	N-CA-CB	-11.38	90.13	110.60
1	A	374	ARG	NE-CZ-NH1	-11.25	114.67	120.30
1	A	17	ILE	N-CA-CB	11.21	136.59	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	ARG	CD-NE-CZ	11.15	139.21	123.60
1	A	376	GLU	CA-CB-CG	11.07	137.75	113.40
1	A	134	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	A	159	TYR	CA-C-N	10.96	141.31	117.20
1	A	245	ALA	CB-CA-C	10.59	125.99	110.10
1	A	374	ARG	NH1-CZ-NH2	10.59	131.05	119.40
1	A	193	CYS	CA-C-O	10.46	142.08	120.10
1	A	207	GLN	CB-CG-CD	10.32	138.43	111.60
1	A	159	TYR	CA-C-O	-10.21	98.66	120.10
1	A	23	ASP	N-CA-CB	10.21	128.97	110.60
1	A	347	ASN	CA-CB-CG	10.19	135.82	113.40
1	A	281	ASP	CB-CG-OD1	-10.16	109.16	118.30
1	A	377	PHE	N-CA-CB	10.12	128.82	110.60
1	A	36	GLU	CA-CB-CG	9.96	135.32	113.40
1	A	219	LEU	CA-CB-CG	9.95	138.19	115.30
1	A	322	GLU	CA-CB-CG	9.85	135.06	113.40
1	A	33	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	A	40	LYS	N-CA-CB	9.81	128.25	110.60
1	A	71	ASN	N-CA-CB	9.69	128.04	110.60
1	A	292	ARG	NE-CZ-NH1	-9.63	115.48	120.30
1	A	19	ALA	CB-CA-C	9.51	124.37	110.10
1	A	329	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	374	ARG	N-CA-CB	-9.38	93.72	110.60
1	A	41	ILE	N-CA-CB	9.31	132.21	110.80
1	A	127	ALA	N-CA-CB	9.29	123.11	110.10
1	A	332	ARG	CD-NE-CZ	9.25	136.55	123.60
1	A	37	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	173	ALA	CB-CA-C	9.04	123.66	110.10
1	A	187	VAL	N-CA-CB	9.03	131.36	111.50
1	A	160	ALA	N-CA-CB	9.01	122.72	110.10
1	A	104	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	A	249	GLU	N-CA-CB	8.83	126.49	110.60
1	A	235	GLU	N-CA-CB	8.63	126.13	110.60
1	A	33	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	43	LEU	CB-CA-C	8.61	126.56	110.20
1	A	190	HIS	C-N-CA	8.60	140.37	122.30
1	A	376	GLU	CA-C-O	8.60	138.17	120.10
1	A	403	ALA	C-N-CA	8.56	143.11	121.70
1	A	393	THR	CA-CB-CG2	8.56	124.38	112.40
1	A	69	LEU	CB-CA-C	8.53	126.41	110.20
1	A	349	ASP	OD1-CG-OD2	-8.51	107.13	123.30
1	A	309	ILE	N-CA-CB	8.51	130.37	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	398	ALA	CB-CA-C	8.46	122.80	110.10
1	A	266	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	A	142	TRP	CB-CA-C	8.35	127.11	110.40
1	A	47	VAL	N-CA-CB	-8.35	93.14	111.50
1	A	125	PHE	N-CA-CB	8.34	125.61	110.60
1	A	204	GLU	CA-CB-CG	8.27	131.59	113.40
1	A	155	GLU	CG-CD-OE1	8.22	134.74	118.30
1	A	41	ILE	O-C-N	8.17	135.77	122.70
1	A	372	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	291	ILE	CB-CA-C	-8.13	95.33	111.60
1	A	320	GLU	N-CA-CB	8.03	125.06	110.60
1	A	20	ALA	N-CA-C	8.02	132.64	111.00
1	A	231	ARG	CB-CA-C	-7.99	94.42	110.40
1	A	240	LEU	CA-CB-CG	7.87	133.41	115.30
1	A	325	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	342	GLN	N-CA-CB	7.84	124.71	110.60
1	A	101	LEU	CA-CB-CG	7.81	133.25	115.30
1	A	193	CYS	CB-CA-C	7.80	126.00	110.40
1	A	313	ASP	CB-CG-OD1	-7.77	111.30	118.30
1	A	221	LEU	N-CA-CB	7.75	125.89	110.40
1	A	265	GLU	CA-CB-CG	7.73	130.40	113.40
1	A	298	PRO	N-CA-C	7.71	132.15	112.10
1	A	101	LEU	CB-CG-CD2	7.62	123.96	111.00
1	A	70	GLU	N-CA-CB	7.59	124.27	110.60
1	A	42	ASN	N-CA-CB	7.57	124.22	110.60
1	A	161	TYR	CA-CB-CG	7.55	127.75	113.40
1	A	44	GLY	N-CA-C	-7.54	94.24	113.10
1	A	236	ASP	CB-CG-OD2	7.50	125.05	118.30
1	A	21	PRO	C-N-CA	7.42	140.24	121.70
1	A	206	TRP	CB-CA-C	7.40	125.19	110.40
1	A	355	LYS	N-CA-CB	7.37	123.87	110.60
1	A	348	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	322	GLU	CB-CG-CD	7.34	134.02	114.20
1	A	190	HIS	CA-CB-CG	7.33	126.06	113.60
1	A	340	THR	CA-CB-OG1	-7.30	93.67	109.00
1	A	407	VAL	CB-CA-C	7.29	125.26	111.40
1	A	389	VAL	CB-CA-C	7.28	125.24	111.40
1	A	207	GLN	CA-CB-CG	7.25	129.35	113.40
1	A	250	LEU	CA-CB-CG	7.24	131.96	115.30
1	A	234	GLU	CA-C-O	-7.20	104.97	120.10
1	A	309	ILE	CB-CA-C	-7.19	97.22	111.60
1	A	303	ALA	CB-CA-C	-7.17	99.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	PHE	O-C-N	7.14	134.13	122.70
1	A	307	ALA	CB-CA-C	7.12	120.78	110.10
1	A	231	ARG	N-CA-C	7.12	130.21	111.00
1	A	343	GLU	CB-CA-C	-7.04	96.31	110.40
1	A	289	ALA	CB-CA-C	7.04	120.66	110.10
1	A	163	ASP	CB-CA-C	7.04	124.48	110.40
1	A	193	CYS	O-C-N	-7.03	111.46	122.70
1	A	393	THR	CA-CB-OG1	-7.02	94.25	109.00
1	A	255	SER	N-CA-CB	7.02	121.03	110.50
1	A	120	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	200	ASP	N-CA-C	6.98	129.84	111.00
1	A	300	ALA	CB-CA-C	-6.98	99.63	110.10
1	A	362	PHE	CB-CA-C	6.94	124.28	110.40
1	A	309	ILE	CA-CB-CG1	6.93	124.17	111.00
1	A	209	LEU	CA-CB-CG	6.91	131.19	115.30
1	A	90	THR	C-N-CA	6.86	138.85	121.70
1	A	26	LEU	N-CA-CB	6.80	124.00	110.40
1	A	389	VAL	CA-CB-CG1	6.79	121.08	110.90
1	A	76	ASN	CA-CB-CG	6.76	128.28	113.40
1	A	100	ALA	N-CA-CB	6.75	119.56	110.10
1	A	343	GLU	OE1-CD-OE2	6.69	131.32	123.30
1	A	132	VAL	CB-CA-C	6.68	124.10	111.40
1	A	146	LYS	CA-CB-CG	6.67	128.07	113.40
1	A	294	ASN	N-CA-CB	6.63	122.54	110.60
1	A	193	CYS	CA-CB-SG	-6.62	102.08	114.00
1	A	211	GLN	CB-CG-CD	6.59	128.74	111.60
1	A	376	GLU	CG-CD-OE1	6.59	131.49	118.30
1	A	396	ASN	N-CA-CB	6.57	122.42	110.60
1	A	126	LEU	CB-CA-C	6.56	122.66	110.20
1	A	384	SER	N-CA-CB	6.56	120.33	110.50
1	A	288	LYS	N-CA-CB	6.55	122.39	110.60
1	A	20	ALA	N-CA-CB	-6.54	100.95	110.10
1	A	91	GLN	CA-CB-CG	6.49	127.67	113.40
1	A	396	ASN	O-C-N	6.48	133.07	122.70
1	A	236	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	A	402	GLU	CA-CB-CG	6.48	127.65	113.40
1	A	49	LYS	O-C-N	6.47	133.06	122.70
1	A	37	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	44	GLY	CA-C-O	6.46	132.23	120.60
1	A	234	GLU	CA-C-N	6.46	131.40	117.20
1	A	278	GLU	CB-CG-CD	6.43	131.56	114.20
1	A	51	GLU	CB-CG-CD	6.42	131.54	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	GLU	C-N-CA	6.40	137.70	121.70
1	A	121	VAL	CB-CA-C	6.39	123.55	111.40
1	A	322	GLU	N-CA-CB	6.39	122.11	110.60
1	A	247	HIS	N-CA-C	6.37	128.19	111.00
1	A	355	LYS	C-N-CA	6.36	137.60	121.70
1	A	327	ARG	N-CA-CB	6.33	122.00	110.60
1	A	280	VAL	CB-CA-C	6.31	123.40	111.40
1	A	72	GLU	N-CA-CB	6.31	121.96	110.60
1	A	356	GLN	C-N-CA	6.31	137.48	121.70
1	A	166	ASN	CB-CA-C	6.30	123.00	110.40
1	A	222	PHE	O-C-N	6.30	132.78	122.70
1	A	43	LEU	N-CA-C	-6.29	94.01	111.00
1	A	25	ILE	N-CA-CB	-6.29	96.33	110.80
1	A	159	TYR	CB-CA-C	6.27	122.95	110.40
1	A	72	GLU	C-N-CA	6.26	137.35	121.70
1	A	80	ILE	CB-CA-C	-6.25	99.09	111.60
1	A	22	ALA	N-CA-C	6.22	127.79	111.00
1	A	142	TRP	N-CA-C	-6.22	94.21	111.00
1	A	126	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	334	ARG	NH1-CZ-NH2	-6.18	112.60	119.40
1	A	340	THR	CB-CA-C	6.18	128.29	111.60
1	A	342	GLN	CB-CG-CD	6.18	127.66	111.60
1	A	349	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	209	LEU	N-CA-CB	-6.11	98.17	110.40
1	A	71	ASN	CA-CB-CG	6.11	126.83	113.40
1	A	169	LEU	N-CA-CB	-6.10	98.19	110.40
1	A	260	PHE	CA-CB-CG	6.10	128.54	113.90
1	A	59	THR	N-CA-CB	6.10	121.89	110.30
1	A	157	ARG	CD-NE-CZ	6.09	132.12	123.60
1	A	357	ASN	N-CA-C	6.08	127.42	111.00
1	A	50	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	68	LEU	CA-CB-CG	6.06	129.23	115.30
1	A	116	THR	CA-CB-CG2	6.04	120.86	112.40
1	A	238	GLU	CB-CA-C	-6.04	98.32	110.40
1	A	169	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	374	ARG	CA-CB-CG	6.02	126.64	113.40
1	A	200	ASP	CB-CA-C	-6.01	98.38	110.40
1	A	135	VAL	CA-CB-CG1	6.00	119.91	110.90
1	A	326	MET	CB-CA-C	6.00	122.40	110.40
1	A	344	LYS	N-CA-CB	5.96	121.32	110.60
1	A	165	GLU	CA-C-N	5.95	130.30	117.20
1	A	23	ASP	OD1-CG-OD2	-5.95	111.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	296	SER	CA-C-O	-5.94	107.63	120.10
1	A	376	GLU	C-N-CA	5.93	136.53	121.70
1	A	210	ALA	O-C-N	5.91	132.16	122.70
1	A	49	LYS	CA-C-O	-5.89	107.73	120.10
1	A	23	ASP	N-CA-C	-5.88	95.12	111.00
1	A	332	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	218	TRP	N-CA-C	5.88	126.88	111.00
1	A	235	GLU	CB-CG-CD	5.88	130.07	114.20
1	A	189	PHE	CB-CA-C	5.87	122.15	110.40
1	A	393	THR	N-CA-CB	-5.86	99.16	110.30
1	A	208	THR	C-N-CA	5.85	136.32	121.70
1	A	162	TYR	N-CA-CB	5.84	121.12	110.60
1	A	346	ALA	CB-CA-C	5.83	118.84	110.10
1	A	376	GLU	CB-CA-C	5.83	122.06	110.40
1	A	158	GLU	CB-CG-CD	5.82	129.91	114.20
1	A	336	LEU	N-CA-CB	-5.82	98.77	110.40
1	A	265	GLU	C-N-CA	5.79	136.17	121.70
1	A	325	ASP	O-C-N	5.79	131.96	122.70
1	A	93	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	357	ASN	CA-CB-CG	5.77	126.10	113.40
1	A	158	GLU	CB-CA-C	5.76	121.93	110.40
1	A	262	LEU	N-CA-C	5.76	126.55	111.00
1	A	348	ARG	C-N-CA	5.75	136.07	121.70
1	A	103	ASN	CB-CA-C	5.74	121.88	110.40
1	A	171	PHE	CA-C-N	-5.73	104.59	117.20
1	A	386	ARG	CD-NE-CZ	5.73	131.63	123.60
1	A	15	GLU	OE1-CD-OE2	-5.72	116.43	123.30
1	A	142	TRP	N-CA-CB	5.70	120.86	110.60
1	A	189	PHE	CA-CB-CG	5.69	127.57	113.90
1	A	165	GLU	CA-C-O	-5.69	108.14	120.10
1	A	60	SER	CB-CA-C	5.69	120.91	110.10
1	A	166	ASN	N-CA-CB	5.68	120.83	110.60
1	A	14	PHE	CB-CG-CD1	5.68	124.78	120.80
1	A	178	LEU	O-C-N	5.67	131.77	122.70
1	A	72	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	A	129	ASN	N-CA-CB	5.66	120.79	110.60
1	A	77	TYR	O-C-N	5.65	131.74	122.70
1	A	252	VAL	CB-CA-C	5.65	122.13	111.40
1	A	190	HIS	N-CA-CB	5.65	120.76	110.60
1	A	81	ASP	CB-CA-C	5.64	121.67	110.40
1	A	176	ASN	O-C-N	5.64	131.72	122.70
1	A	328	GLN	N-CA-CB	5.63	120.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	372	ARG	CB-CA-C	-5.62	99.16	110.40
1	A	245	ALA	CA-C-O	5.61	131.88	120.10
1	A	303	ALA	O-C-N	5.60	131.67	122.70
1	A	15	GLU	CB-CG-CD	5.60	129.32	114.20
1	A	70	GLU	CG-CD-OE2	-5.57	107.16	118.30
1	A	293	ALA	CA-C-O	-5.57	108.41	120.10
1	A	372	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	118	ALA	O-C-N	5.57	131.61	122.70
1	A	204	GLU	CG-CD-OE2	-5.51	107.28	118.30
1	A	341	LEU	CB-CA-C	5.50	120.66	110.20
1	A	149	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	A	31	LEU	CB-CA-C	5.50	120.65	110.20
1	A	320	GLU	CA-CB-CG	5.49	125.49	113.40
1	A	347	ASN	N-CA-CB	-5.49	100.71	110.60
1	A	376	GLU	OE1-CD-OE2	-5.49	116.72	123.30
1	A	332	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	28	LEU	N-CA-CB	5.45	121.29	110.40
1	A	281	ASP	C-N-CA	5.44	135.30	121.70
1	A	103	ASN	CA-C-N	-5.44	105.24	117.20
1	A	340	THR	N-CA-CB	-5.43	99.98	110.30
1	A	291	ILE	O-C-N	5.43	131.39	122.70
1	A	343	GLU	CG-CD-OE2	-5.43	107.44	118.30
1	A	386	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
1	A	88	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	104	ASP	CA-C-N	-5.41	105.30	117.20
1	A	18	THR	CA-CB-OG1	-5.41	97.65	109.00
1	A	111	GLN	CB-CG-CD	-5.39	97.57	111.60
1	A	234	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	A	396	ASN	CB-CA-C	-5.38	99.65	110.40
1	A	181	ALA	C-N-CA	5.37	135.13	121.70
1	A	89	CYS	N-CA-CB	5.37	120.26	110.60
1	A	300	ALA	N-CA-C	5.37	125.48	111.00
1	A	144	ASN	CA-CB-CG	5.34	125.16	113.40
1	A	325	ASP	CA-C-N	-5.34	105.44	117.20
1	A	244	ALA	CB-CA-C	5.34	118.11	110.10
1	A	85	GLU	N-CA-C	-5.33	96.60	111.00
1	A	378	GLY	CA-C-O	5.33	130.19	120.60
1	A	204	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	A	353	ILE	N-CA-CB	5.33	123.05	110.80
1	A	230	ALA	N-CA-CB	-5.32	102.66	110.10
1	A	403	ALA	CA-C-O	5.32	131.27	120.10
1	A	85	GLU	N-CA-CB	5.31	120.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	105	LYS	N-CA-C	-5.31	96.67	111.00
1	A	166	ASN	N-CA-C	-5.31	96.67	111.00
1	A	355	LYS	CA-C-O	5.30	131.24	120.10
1	A	210	ALA	N-CA-CB	5.30	117.51	110.10
1	A	44	GLY	CA-C-N	-5.29	105.57	117.20
1	A	264	ASN	N-CA-CB	-5.28	101.09	110.60
1	A	216	LYS	CB-CA-C	5.28	120.96	110.40
1	A	215	GLU	N-CA-CB	5.28	120.10	110.60
1	A	194	HIS	N-CA-CB	-5.28	101.10	110.60
1	A	238	GLU	N-CA-C	-5.26	96.80	111.00
1	A	21	PRO	O-C-N	-5.26	114.29	122.70
1	A	238	GLU	N-CA-CB	5.26	120.06	110.60
1	A	309	ILE	O-C-N	5.25	131.10	122.70
1	A	125	PHE	N-CA-C	-5.25	96.84	111.00
1	A	206	TRP	N-CA-C	-5.24	96.85	111.00
1	A	43	LEU	CA-C-O	5.23	131.07	120.10
1	A	180	GLU	CA-C-N	5.22	128.69	117.20
1	A	155	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	A	123	ALA	N-CA-CB	-5.20	102.81	110.10
1	A	51	GLU	CA-CB-CG	5.20	124.83	113.40
1	A	42	ASN	O-C-N	5.18	130.99	122.70
1	A	93	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	A	198	GLY	C-N-CA	5.18	134.65	121.70
1	A	18	THR	CB-CA-C	5.18	125.58	111.60
1	A	402	GLU	N-CA-CB	5.18	119.92	110.60
1	A	90	THR	CA-C-O	5.17	130.95	120.10
1	A	18	THR	N-CA-C	-5.17	97.05	111.00
1	A	248	LYS	N-CA-CB	5.16	119.89	110.60
1	A	171	PHE	C-N-CA	5.15	134.59	121.70
1	A	233	LEU	C-N-CA	5.15	134.58	121.70
1	A	246	MET	CA-CB-CG	5.15	122.06	113.30
1	A	58	LEU	N-CA-C	5.15	124.90	111.00
1	A	193	CYS	CA-C-N	-5.12	105.94	117.20
1	A	114	GLY	N-CA-C	5.11	125.88	113.10
1	A	19	ALA	N-CA-C	-5.11	97.21	111.00
1	A	277	SER	N-CA-CB	5.10	118.16	110.50
1	A	35	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	348	ARG	CD-NE-CZ	-5.07	116.50	123.60
1	A	26	LEU	C-N-CA	5.07	132.94	122.30
1	A	264	ASN	C-N-CA	5.07	134.37	121.70
1	A	371	LEU	CB-CG-CD2	5.07	119.61	111.00
1	A	196	PRO	CB-CA-C	-5.06	99.35	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	GLU	CG-CD-OE2	-5.05	108.19	118.30
1	A	210	ALA	CA-C-O	-5.04	109.53	120.10
1	A	255	SER	CA-C-N	-5.03	106.14	117.20
1	A	312	ASN	N-CA-CB	5.02	119.63	110.60
1	A	106	ARG	CD-NE-CZ	-5.01	116.58	123.60
1	A	276	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain
1	A	120	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	241	ARG	Sidechain
1	A	266	ARG	Sidechain
1	A	292	ARG	Sidechain
1	A	316	ARG	Sidechain
1	A	327	ARG	Sidechain
1	A	348	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	A	3065	0	3008	669	12
2	A	5	0	0	0	0
3	A	16	0	10	6	0
All	All	3086	0	3018	670	12

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 110.

All (670) 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:A:199:ILE:O	1:A:200:ASP:HB3	1.38	1.20
1:A:202:THR:N	1:A:205:GLN:HE21	1.39	1.19
1:A:202:THR:H	1:A:205:GLN:NE2	1.42	1.16
1:A:198:GLY:HA3	1:A:357:ASN:O	1.49	1.09
1:A:26:LEU:HD22	1:A:29:ALA:HB3	1.34	1.08
1:A:146:LYS:HB2	1:A:156:VAL:HG21	1.35	1.07
1:A:47:VAL:HG13	1:A:55:THR:HG21	1.30	1.07
1:A:116:THR:HB	1:A:142:TRP:HH2	1.19	1.06
1:A:128:LYS:HZ3	1:A:286:GLN:HB3	1.20	1.04
1:A:74:THR:O	1:A:75:LYS:HB3	1.49	1.04
1:A:37:ARG:HB2	1:A:38:PRO:HD2	1.40	1.01
1:A:59:THR:O	1:A:61:VAL:N	1.94	1.01
1:A:61:VAL:HG12	1:A:309:ILE:HD11	1.42	1.01
1:A:338:VAL:HG11	1:A:354:ILE:HD11	1.43	1.00
1:A:20:ALA:HB3	1:A:21:PRO:HD3	1.42	1.00
1:A:104:ASP:HB3	1:A:106:ARG:HG2	1.38	0.99
1:A:26:LEU:CD2	1:A:29:ALA:HB3	1.92	0.99
1:A:335:GLN:HA	1:A:354:ILE:CG2	1.94	0.98
1:A:263:TYR:O	1:A:265:GLU:N	1.96	0.98
1:A:74:THR:HG23	1:A:75:LYS:H	1.27	0.97
1:A:312:ASN:O	1:A:316:ARG:HB2	1.67	0.95
1:A:51:GLU:N	1:A:329:ARG:HH12	1.65	0.93
1:A:41:ILE:HG22	1:A:43:LEU:HD12	1.47	0.92
1:A:172:ASP:O	1:A:176:ASN:ND2	2.02	0.91
1:A:125:PHE:O	1:A:128:LYS:HG3	1.69	0.91
1:A:42:ASN:HA	1:A:380:TYR:HB2	1.53	0.91
1:A:57:VAL:O	1:A:58:LEU:HB2	1.71	0.90
1:A:128:LYS:O	1:A:130:THR:N	2.05	0.90
1:A:197:THR:O	1:A:199:ILE:N	2.05	0.89
1:A:54:LYS:O	1:A:56:PRO:HD3	1.72	0.89
1:A:192:CYS:HB3	1:A:231:ARG:NH1	1.88	0.89
1:A:47:VAL:CG1	1:A:55:THR:HG21	2.04	0.88
1:A:112:THR:HG21	1:A:118:ALA:HB2	1.55	0.88
1:A:128:LYS:HE3	1:A:129:ASN:N	1.89	0.88
1:A:27:GLY:C	1:A:28:LEU:HD22	1.94	0.87
1:A:40:LYS:C	1:A:40:LYS:HZ2	1.76	0.87
1:A:45:ILE:CG2	1:A:47:VAL:H	1.87	0.86
1:A:327:ARG:HG2	1:A:327:ARG:HH11	1.40	0.86
1:A:64:ALA:O	1:A:68:LEU:HD13	1.76	0.86
1:A:82:GLY:HA3	1:A:111:GLN:HB2	1.58	0.85
1:A:220:PRO:HD3	1:A:247:HIS:CE1	2.11	0.85
1:A:144:ASN:O	1:A:148:VAL:HG13	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HD21	1:A:392:MET:HG3	1.58	0.84
1:A:48:TYR:CZ	1:A:326:MET:HG3	2.13	0.84
1:A:221:LEU:O	1:A:222:PHE:HB2	1.77	0.84
1:A:329:ARG:O	1:A:333:MET:HB2	1.77	0.83
1:A:116:THR:HB	1:A:142:TRP:CH2	2.11	0.83
1:A:80:ILE:HD12	1:A:288:LYS:HB3	1.60	0.83
1:A:40:LYS:HE3	1:A:400:LEU:HD22	1.58	0.82
1:A:175:ILE:O	1:A:179:ASN:HB3	1.80	0.82
1:A:335:GLN:HA	1:A:354:ILE:HG23	1.58	0.82
1:A:48:TYR:O	1:A:49:LYS:HG3	1.80	0.82
1:A:335:GLN:HA	1:A:354:ILE:HG21	1.61	0.81
1:A:228:GLY:HA3	1:A:233:LEU:HD12	1.61	0.81
1:A:365:LEU:HB3	1:A:369:GLN:HB3	1.63	0.81
1:A:39:GLY:O	1:A:41:ILE:N	2.14	0.81
1:A:230:ALA:HB1	1:A:357:ASN:OD1	1.79	0.81
1:A:36:GLU:O	1:A:37:ARG:HB3	1.79	0.81
1:A:109:THR:HB	1:A:271:THR:HB	1.61	0.81
1:A:50:ASP:C	1:A:52:THR:H	1.84	0.80
1:A:100:ALA:O	1:A:104:ASP:N	2.15	0.80
1:A:68:LEU:O	1:A:72:GLU:HB2	1.81	0.80
1:A:58:LEU:O	1:A:59:THR:HG22	1.82	0.79
1:A:338:VAL:CG1	1:A:354:ILE:HD11	2.12	0.79
1:A:135:VAL:O	1:A:156:VAL:HA	1.81	0.79
1:A:111:GLN:NE2	1:A:303:ALA:HB2	1.99	0.78
1:A:40:LYS:O	1:A:40:LYS:NZ	2.15	0.78
1:A:388:ASN:ND2	1:A:390:ALA:HB3	1.98	0.78
1:A:128:LYS:HD2	1:A:286:GLN:HG2	1.64	0.78
1:A:42:ASN:HA	1:A:380:TYR:CB	2.13	0.78
1:A:50:ASP:OD1	1:A:52:THR:HB	1.83	0.78
1:A:142:TRP:O	1:A:145:HIS:HB2	1.84	0.78
1:A:116:THR:HG22	3:A:1:PMP:H5A1	1.65	0.77
1:A:152:ALA:O	1:A:154:LEU:N	2.16	0.77
1:A:296:SER:O	1:A:297:ASN:ND2	2.16	0.77
1:A:276:ASP:HB2	1:A:279:THR:H	1.49	0.77
1:A:121:VAL:CG2	1:A:291:ILE:HD13	2.15	0.77
1:A:124:ASP:OD1	1:A:124:ASP:N	2.14	0.77
1:A:115:GLY:HA3	3:A:1:PMP:H5A2	1.66	0.76
1:A:210:ALA:HB2	1:A:243:PHE:CE1	2.19	0.76
1:A:404:ILE:O	1:A:407:VAL:HG22	1.84	0.76
1:A:30:ASP:O	1:A:32:PHE:N	2.19	0.76
1:A:235:GLU:HG3	1:A:235:GLU:O	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PHE:HD2	1:A:356:GLN:HE22	1.30	0.76
1:A:106:ARG:NE	1:A:274:ALA:O	2.18	0.76
1:A:45:ILE:HG22	1:A:47:VAL:H	1.50	0.76
1:A:310:LEU:O	1:A:316:ARG:NH1	2.19	0.76
1:A:348:ARG:NH2	1:A:348:ARG:HG3	2.01	0.76
1:A:130:THR:CG2	1:A:132:VAL:HB	2.16	0.75
1:A:144:ASN:HD22	1:A:148:VAL:CG1	1.99	0.75
1:A:59:THR:O	1:A:62:LYS:N	2.16	0.75
1:A:67:TYR:HD1	1:A:68:LEU:HD12	1.51	0.75
1:A:23:ASP:OD2	1:A:25:ILE:HB	1.86	0.75
1:A:366:THR:O	1:A:368:GLU:N	2.18	0.75
1:A:182:GLN:O	1:A:185:ASP:HB2	1.87	0.74
1:A:392:MET:HG2	1:A:400:LEU:HD21	1.68	0.74
1:A:35:ASP:O	1:A:37:ARG:NH2	2.21	0.74
1:A:28:LEU:HD21	1:A:381:ALA:O	1.88	0.74
1:A:341:LEU:HD23	1:A:401:CYS:SG	2.26	0.74
1:A:84:PRO:HA	1:A:87:GLY:HA3	1.69	0.74
1:A:339:ASN:HD22	1:A:339:ASN:C	1.89	0.74
1:A:202:THR:OG1	1:A:205:GLN:HG3	1.86	0.74
1:A:112:THR:HG22	1:A:269:ALA:HA	1.70	0.74
1:A:86:PHE:HE2	1:A:269:ALA:HB2	1.50	0.74
1:A:394:PRO:HG2	1:A:395:ASP:H	1.53	0.73
1:A:135:VAL:HA	1:A:186:VAL:O	1.89	0.73
1:A:49:LYS:HB3	1:A:53:GLY:HA2	1.72	0.72
1:A:221:LEU:O	1:A:251:ILE:O	2.06	0.72
1:A:396:ASN:HD22	1:A:396:ASN:N	1.86	0.72
1:A:150:ASN:OD1	1:A:155:GLU:HG2	1.90	0.72
1:A:110:ALA:O	1:A:269:ALA:HB1	1.90	0.72
1:A:40:LYS:HZ1	1:A:396:ASN:CG	1.93	0.71
1:A:365:LEU:N	1:A:365:LEU:HD22	2.05	0.71
1:A:365:LEU:CD2	1:A:365:LEU:N	2.54	0.71
1:A:47:VAL:HG13	1:A:55:THR:CG2	2.15	0.71
1:A:165:GLU:O	1:A:166:ASN:C	2.28	0.71
1:A:237:ALA:O	1:A:241:ARG:HB3	1.91	0.71
1:A:45:ILE:CG2	1:A:47:VAL:O	2.39	0.71
1:A:167:HIS:O	1:A:168:THR:HG23	1.90	0.71
1:A:241:ARG:O	1:A:244:ALA:N	2.20	0.71
1:A:41:ILE:HG23	1:A:42:ASN:N	2.05	0.70
1:A:312:ASN:O	1:A:316:ARG:N	2.25	0.70
1:A:30:ASP:C	1:A:32:PHE:N	2.43	0.70
1:A:74:THR:CG2	1:A:75:LYS:H	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HG23	1:A:47:VAL:H	1.56	0.70
1:A:128:LYS:NZ	1:A:286:GLN:HB3	2.02	0.70
1:A:372:ARG:O	1:A:375:GLU:HB3	1.92	0.69
1:A:58:LEU:HD22	1:A:260:PHE:O	1.93	0.69
1:A:26:LEU:O	1:A:28:LEU:N	2.25	0.69
1:A:404:ILE:HA	1:A:407:VAL:HG22	1.73	0.69
1:A:314:ALA:O	1:A:318:ILE:HG13	1.92	0.69
1:A:122:ALA:O	1:A:126:LEU:HB2	1.93	0.69
1:A:134:ARG:HB2	1:A:155:GLU:O	1.92	0.69
1:A:229:PHE:HE1	1:A:326:MET:HG2	1.55	0.69
1:A:59:THR:HG23	1:A:60:SER:H	1.57	0.69
1:A:74:THR:HG23	1:A:75:LYS:N	2.06	0.69
1:A:165:GLU:O	1:A:167:HIS:N	2.25	0.69
1:A:47:VAL:HG22	1:A:263:TYR:OH	1.93	0.68
1:A:365:LEU:O	1:A:367:LYS:N	2.26	0.68
1:A:199:ILE:HG22	1:A:200:ASP:H	1.58	0.68
1:A:375:GLU:C	1:A:377:PHE:H	1.96	0.68
1:A:327:ARG:NH1	1:A:327:ARG:HG2	2.09	0.68
1:A:256:TYR:HD2	1:A:260:PHE:CE2	2.11	0.68
1:A:315:LEU:HD12	1:A:318:ILE:HD12	1.76	0.68
1:A:30:ASP:C	1:A:32:PHE:H	1.97	0.68
1:A:373:LEU:O	1:A:377:PHE:HB2	1.94	0.68
1:A:67:TYR:CD1	1:A:68:LEU:HD12	2.29	0.68
1:A:190:HIS:HA	1:A:223:ASP:O	1.94	0.68
1:A:306:VAL:O	1:A:310:LEU:HB2	1.94	0.68
1:A:45:ILE:HG21	1:A:47:VAL:O	1.94	0.67
1:A:50:ASP:O	1:A:53:GLY:N	2.27	0.67
1:A:136:TRP:CE3	1:A:157:ARG:HB3	2.29	0.67
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.77	0.67
1:A:103:ASN:ND2	1:A:105:LYS:HG2	2.08	0.67
1:A:140:PRO:HG2	1:A:194:HIS:HE1	1.60	0.67
1:A:51:GLU:N	1:A:329:ARG:NH1	2.40	0.67
1:A:370:VAL:HG13	1:A:381:ALA:HB3	1.77	0.67
1:A:13:MET:N	1:A:13:MET:SD	2.68	0.67
1:A:262:LEU:O	1:A:263:TYR:O	2.13	0.67
1:A:14:PHE:C	1:A:14:PHE:CD1	2.69	0.67
1:A:231:ARG:NE	1:A:235:GLU:HG2	2.10	0.66
1:A:315:LEU:HA	1:A:318:ILE:HD12	1.78	0.66
1:A:372:ARG:O	1:A:375:GLU:HG2	1.94	0.66
1:A:87:GLY:O	1:A:91:GLN:HB2	1.95	0.66
1:A:20:ALA:CB	1:A:21:PRO:HD3	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ALA:HB2	1:A:243:PHE:CD1	2.30	0.66
1:A:178:LEU:HD23	1:A:218:TRP:CH2	2.31	0.66
1:A:192:CYS:C	1:A:193:CYS:SG	2.72	0.65
1:A:309:ILE:O	1:A:309:ILE:HG22	1.95	0.65
1:A:229:PHE:HE2	1:A:359:MET:HE1	1.61	0.65
1:A:373:LEU:HG	1:A:379:VAL:HG22	1.76	0.65
1:A:112:THR:CG2	1:A:118:ALA:HB2	2.26	0.65
1:A:276:ASP:O	1:A:280:VAL:HG12	1.97	0.65
1:A:348:ARG:HH21	1:A:348:ARG:HG3	1.61	0.65
1:A:145:HIS:O	1:A:149:PHE:HB2	1.95	0.65
1:A:367:LYS:HD3	1:A:368:GLU:OE1	1.96	0.65
1:A:276:ASP:HB2	1:A:279:THR:OG1	1.97	0.65
1:A:192:CYS:HG	1:A:236:ASP:CG	1.99	0.65
1:A:232:GLY:H	1:A:327:ARG:NH1	1.95	0.65
1:A:126:LEU:HD12	1:A:130:THR:OG1	1.96	0.65
1:A:393:THR:HG23	1:A:394:PRO:HD2	1.78	0.65
1:A:116:THR:CB	1:A:142:TRP:HH2	2.04	0.64
1:A:128:LYS:CD	1:A:286:GLN:HG2	2.27	0.64
1:A:28:LEU:N	1:A:28:LEU:HD22	2.12	0.64
1:A:334:ARG:NH2	1:A:360:PHE:O	2.31	0.64
1:A:231:ARG:CZ	1:A:235:GLU:HG2	2.27	0.64
1:A:256:TYR:O	1:A:260:PHE:HB2	1.98	0.63
1:A:315:LEU:CD1	1:A:318:ILE:HD12	2.29	0.63
1:A:150:ASN:OD1	1:A:155:GLU:CG	2.45	0.63
1:A:194:HIS:HB3	1:A:197:THR:O	1.99	0.63
1:A:203:LEU:O	1:A:207:GLN:HB2	1.98	0.63
1:A:43:LEU:HD11	1:A:391:GLY:C	2.19	0.63
1:A:330:ILE:O	1:A:334:ARG:HB2	1.99	0.63
1:A:382:VAL:CG1	1:A:386:ARG:HB3	2.29	0.63
1:A:396:ASN:O	1:A:397:MET:C	2.37	0.63
1:A:327:ARG:CG	1:A:327:ARG:HH11	2.10	0.62
1:A:396:ASN:HD22	1:A:396:ASN:H	1.47	0.62
1:A:197:THR:O	1:A:197:THR:OG1	2.16	0.62
1:A:125:PHE:CD1	1:A:128:LYS:HE2	2.34	0.62
1:A:339:ASN:O	1:A:339:ASN:ND2	2.33	0.62
1:A:327:ARG:CG	1:A:327:ARG:NH1	2.61	0.62
1:A:337:PHE:CD1	1:A:392:MET:CE	2.82	0.62
1:A:14:PHE:HD1	1:A:14:PHE:C	2.02	0.62
1:A:382:VAL:HG13	1:A:382:VAL:O	1.98	0.62
1:A:148:VAL:HG23	1:A:148:VAL:O	1.97	0.62
1:A:328:GLN:O	1:A:332:ARG:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:NH1	1:A:389:VAL:HG21	2.15	0.62
1:A:402:GLU:HG2	1:A:402:GLU:O	1.99	0.62
1:A:179:ASN:HB2	1:A:216:LYS:CE	2.30	0.62
1:A:179:ASN:HB2	1:A:216:LYS:NZ	2.15	0.62
1:A:232:GLY:N	1:A:327:ARG:NH1	2.48	0.62
1:A:356:GLN:O	1:A:356:GLN:HG2	2.00	0.62
1:A:136:TRP:HZ2	1:A:181:ALA:HB3	1.64	0.61
1:A:103:ASN:HD22	1:A:105:LYS:HG2	1.64	0.61
1:A:309:ILE:HG21	1:A:319:TRP:HB2	1.83	0.61
1:A:226:TYR:CZ	1:A:360:PHE:HE2	2.17	0.61
1:A:367:LYS:O	1:A:370:VAL:N	2.33	0.61
1:A:186:VAL:HG23	1:A:187:VAL:O	2.01	0.61
1:A:335:GLN:CA	1:A:354:ILE:HG23	2.31	0.61
1:A:119:LEU:HD13	1:A:145:HIS:NE2	2.15	0.61
1:A:13:MET:CG	1:A:13:MET:O	2.49	0.61
1:A:169:LEU:HD22	1:A:200:ASP:O	1.99	0.61
1:A:32:PHE:CE1	1:A:39:GLY:HA3	2.36	0.61
1:A:363:SER:HB2	1:A:365:LEU:CD2	2.30	0.61
1:A:101:LEU:HA	1:A:104:ASP:HB2	1.83	0.61
1:A:121:VAL:HG21	1:A:291:ILE:HD13	1.82	0.61
1:A:218:TRP:O	1:A:219:LEU:HB2	2.00	0.60
1:A:13:MET:O	1:A:13:MET:SD	2.59	0.60
1:A:209:LEU:O	1:A:213:SER:N	2.34	0.60
1:A:40:LYS:HE2	1:A:400:LEU:HB2	1.83	0.60
1:A:120:ARG:O	1:A:123:ALA:HB3	2.02	0.60
1:A:135:VAL:HB	1:A:186:VAL:HG22	1.84	0.60
1:A:40:LYS:HD3	1:A:41:ILE:N	2.16	0.60
1:A:363:SER:HB2	1:A:365:LEU:HD23	1.83	0.60
1:A:37:ARG:O	1:A:39:GLY:N	2.34	0.60
1:A:136:TRP:CZ2	1:A:181:ALA:HB3	2.37	0.60
1:A:40:LYS:CG	1:A:41:ILE:N	2.64	0.60
1:A:19:ALA:O	1:A:20:ALA:HB2	2.00	0.60
1:A:113:PRO:HA	1:A:266:ARG:HB2	1.84	0.60
1:A:229:PHE:HE2	1:A:359:MET:CE	2.14	0.59
1:A:40:LYS:CE	1:A:400:LEU:HD22	2.31	0.59
1:A:43:LEU:CD2	1:A:392:MET:HG3	2.31	0.59
1:A:83:ILE:O	1:A:86:PHE:HB3	2.01	0.59
1:A:393:THR:HG23	1:A:394:PRO:CD	2.31	0.59
1:A:119:LEU:O	1:A:122:ALA:HB3	2.02	0.59
1:A:367:LYS:HB2	1:A:368:GLU:OE1	2.03	0.59
1:A:339:ASN:ND2	1:A:339:ASN:C	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:O	1:A:372:ARG:HB3	2.03	0.59
1:A:46:GLY:O	1:A:47:VAL:HG23	2.02	0.59
1:A:40:LYS:HG3	1:A:41:ILE:H	1.68	0.59
1:A:146:LYS:O	1:A:150:ASN:ND2	2.36	0.59
1:A:101:LEU:HD23	1:A:106:ARG:HG3	1.83	0.59
1:A:344:LYS:O	1:A:345:GLY:C	2.40	0.59
1:A:257:SER:HB3	1:A:263:TYR:HD2	1.68	0.58
1:A:49:LYS:CG	1:A:55:THR:HG23	2.33	0.58
1:A:40:LYS:NZ	1:A:396:ASN:OD1	2.27	0.58
1:A:178:LEU:CD2	1:A:218:TRP:CH2	2.86	0.58
1:A:26:LEU:HD23	1:A:29:ALA:HB3	1.82	0.58
1:A:401:CYS:O	1:A:404:ILE:HG22	2.03	0.58
1:A:40:LYS:HG3	1:A:41:ILE:N	2.18	0.58
1:A:128:LYS:HZ3	1:A:286:GLN:CB	2.06	0.58
1:A:312:ASN:HB3	1:A:315:LEU:HB2	1.84	0.58
1:A:37:ARG:CB	1:A:38:PRO:HD2	2.17	0.58
1:A:174:LEU:O	1:A:178:LEU:N	2.30	0.58
1:A:32:PHE:HD1	1:A:380:TYR:CE1	2.22	0.58
1:A:199:ILE:HG22	1:A:200:ASP:N	2.19	0.58
1:A:40:LYS:NZ	1:A:396:ASN:HB3	2.18	0.58
1:A:175:ILE:CD1	1:A:209:LEU:HD12	2.34	0.57
1:A:321:GLN:HE21	1:A:321:GLN:C	2.07	0.57
1:A:336:LEU:O	1:A:337:PHE:C	2.42	0.57
1:A:128:LYS:NZ	1:A:129:ASN:HB2	2.19	0.57
1:A:27:GLY:O	1:A:28:LEU:HD13	2.04	0.57
1:A:375:GLU:CG	1:A:376:GLU:N	2.67	0.57
1:A:389:VAL:O	1:A:392:MET:HB2	2.05	0.57
1:A:202:THR:OG1	1:A:205:GLN:CG	2.52	0.57
1:A:306:VAL:O	1:A:310:LEU:HD22	2.05	0.57
1:A:200:ASP:OD2	1:A:201:PRO:O	2.23	0.57
1:A:119:LEU:HD23	1:A:253:ALA:CB	2.35	0.57
1:A:101:LEU:CA	1:A:104:ASP:HB2	2.35	0.57
1:A:112:THR:HG21	1:A:118:ALA:CB	2.32	0.57
1:A:144:ASN:HD22	1:A:148:VAL:HG12	1.70	0.57
1:A:388:ASN:HD21	1:A:390:ALA:HB3	1.70	0.57
1:A:193:CYS:SG	1:A:357:ASN:ND2	2.77	0.56
1:A:257:SER:O	1:A:258:ALA:HB2	2.05	0.56
1:A:78:LEU:HD22	1:A:300:ALA:HB2	1.87	0.56
1:A:321:GLN:HE22	1:A:325:ASP:CG	2.08	0.56
1:A:171:PHE:O	1:A:174:LEU:HB3	2.03	0.56
1:A:32:PHE:HE1	1:A:39:GLY:HA3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PRO:CG	1:A:196:PRO:HD2	2.36	0.56
1:A:193:CYS:SG	1:A:200:ASP:HB2	2.45	0.56
1:A:73:THR:HG23	1:A:74:THR:HB	1.88	0.56
1:A:119:LEU:HD23	1:A:253:ALA:HB3	1.87	0.56
1:A:399:PRO:O	1:A:403:ALA:N	2.39	0.56
1:A:128:LYS:HE3	1:A:129:ASN:H	1.68	0.56
1:A:185:ASP:O	1:A:218:TRP:O	2.23	0.56
1:A:334:ARG:NH2	1:A:361:SER:OG	2.38	0.56
1:A:104:ASP:O	1:A:105:LYS:HB2	2.05	0.56
1:A:112:THR:CG2	1:A:269:ALA:HA	2.35	0.56
1:A:108:ARG:HB2	1:A:284:PHE:CD1	2.40	0.56
1:A:26:LEU:HD22	1:A:26:LEU:O	2.06	0.56
1:A:394:PRO:CG	1:A:395:ASP:H	2.17	0.56
1:A:84:PRO:O	1:A:88:ARG:HG2	2.05	0.56
1:A:404:ILE:HA	1:A:407:VAL:CG2	2.36	0.56
1:A:321:GLN:NE2	1:A:325:ASP:OD1	2.38	0.56
3:A:1:PMP:H4A2	3:A:1:PMP:O4P	2.04	0.55
1:A:255:SER:OG	3:A:1:PMP:O2P	2.15	0.55
1:A:260:PHE:HE1	1:A:309:ILE:HG13	1.71	0.55
1:A:353:ILE:CG1	1:A:354:ILE:N	2.69	0.55
1:A:111:GLN:CD	1:A:303:ALA:HB2	2.26	0.55
1:A:382:VAL:HG11	1:A:386:ARG:HB3	1.87	0.55
1:A:179:ASN:HB2	1:A:216:LYS:HZ3	1.71	0.55
1:A:232:GLY:HA2	1:A:327:ARG:CZ	2.36	0.55
1:A:41:ILE:CG2	1:A:42:ASN:N	2.68	0.55
1:A:298:PRO:O	1:A:300:ALA:N	2.36	0.55
1:A:152:ALA:C	1:A:154:LEU:H	2.07	0.55
1:A:23:ASP:CG	1:A:24:PRO:HD2	2.27	0.55
1:A:130:THR:HG23	1:A:132:VAL:HB	1.89	0.55
1:A:260:PHE:CE1	1:A:309:ILE:HG13	2.41	0.55
1:A:276:ASP:O	1:A:280:VAL:CG1	2.54	0.55
1:A:210:ALA:C	1:A:212:LEU:N	2.58	0.55
1:A:353:ILE:HG13	1:A:354:ILE:N	2.18	0.55
1:A:173:ALA:O	1:A:177:SER:HB2	2.06	0.55
1:A:128:LYS:O	1:A:129:ASN:C	2.45	0.55
1:A:287:MET:C	1:A:289:ALA:H	2.08	0.55
1:A:220:PRO:HD3	1:A:247:HIS:HE1	1.66	0.54
1:A:238:GLU:O	1:A:239:GLY:C	2.46	0.54
1:A:393:THR:O	1:A:397:MET:N	2.35	0.54
1:A:23:ASP:OD1	1:A:24:PRO:HD2	2.07	0.54
1:A:196:PRO:HG2	1:A:362:PHE:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASN:CG	1:A:17:ILE:H	2.11	0.54
1:A:231:ARG:NH1	1:A:235:GLU:HG2	2.23	0.54
1:A:141:SER:OG	1:A:142:TRP:N	2.35	0.54
1:A:226:TYR:O	1:A:229:PHE:HB3	2.07	0.54
1:A:107:ALA:HB2	1:A:273:VAL:HB	1.89	0.54
1:A:47:VAL:HG22	1:A:263:TYR:CZ	2.43	0.54
1:A:89:CYS:O	1:A:93:LEU:HB2	2.08	0.54
1:A:120:ARG:O	1:A:124:ASP:OD1	2.26	0.54
1:A:192:CYS:SG	1:A:236:ASP:OD2	2.66	0.54
1:A:373:LEU:O	1:A:374:ARG:C	2.46	0.54
1:A:88:ARG:O	1:A:91:GLN:HB3	2.07	0.54
1:A:202:THR:H	1:A:205:GLN:HE21	0.64	0.53
1:A:48:TYR:O	1:A:49:LYS:CG	2.53	0.53
1:A:126:LEU:HD12	1:A:130:THR:CB	2.38	0.53
1:A:241:ARG:HA	1:A:244:ALA:HB3	1.91	0.53
1:A:13:MET:C	1:A:13:MET:SD	2.85	0.53
1:A:234:GLU:O	1:A:236:ASP:N	2.42	0.53
1:A:74:THR:CG2	1:A:75:LYS:N	2.67	0.53
1:A:149:PHE:O	1:A:154:LEU:O	2.26	0.53
1:A:51:GLU:H	1:A:329:ARG:NH1	2.06	0.53
1:A:369:GLN:O	1:A:372:ARG:CB	2.57	0.53
1:A:92:GLU:HG3	1:A:97:LYS:HA	1.91	0.53
1:A:136:TRP:HZ2	1:A:181:ALA:CB	2.21	0.53
1:A:356:GLN:OE1	1:A:361:SER:HB3	2.07	0.53
1:A:128:LYS:HZ1	1:A:129:ASN:HB2	1.74	0.53
1:A:50:ASP:C	1:A:329:ARG:HH12	2.12	0.53
1:A:49:LYS:HG3	1:A:55:THR:HG23	1.91	0.53
1:A:136:TRP:NE1	1:A:185:ASP:OD1	2.42	0.53
1:A:256:TYR:HD1	1:A:268:GLY:HA2	1.72	0.52
1:A:57:VAL:O	1:A:58:LEU:CB	2.50	0.52
1:A:256:TYR:CD2	1:A:260:PHE:CE2	2.96	0.52
1:A:352:PHE:HD2	1:A:356:GLN:NE2	2.05	0.52
1:A:179:ASN:OD1	1:A:180:GLU:N	2.43	0.52
1:A:26:LEU:C	1:A:28:LEU:H	2.13	0.52
1:A:335:GLN:CA	1:A:354:ILE:CG2	2.80	0.52
1:A:272:LEU:C	1:A:273:VAL:HG12	2.29	0.52
1:A:195:ASN:HD22	1:A:196:PRO:HA	1.73	0.52
1:A:20:ALA:CB	1:A:21:PRO:CD	2.88	0.52
1:A:40:LYS:HZ3	1:A:396:ASN:HB3	1.74	0.52
1:A:178:LEU:CD2	1:A:218:TRP:CZ3	2.93	0.52
1:A:261:GLY:O	1:A:262:LEU:HD13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:MET:O	1:A:336:LEU:HB2	2.09	0.52
1:A:43:LEU:HD23	1:A:387:VAL:HG23	1.91	0.52
1:A:141:SER:HG	1:A:142:TRP:H	1.58	0.52
1:A:272:LEU:CD2	1:A:280:VAL:HG23	2.39	0.52
1:A:99:SER:O	1:A:102:ILE:HG22	2.09	0.52
1:A:13:MET:HG2	1:A:13:MET:O	2.10	0.52
1:A:342:GLN:HG2	1:A:342:GLN:O	2.10	0.52
1:A:209:LEU:O	1:A:212:LEU:HB2	2.10	0.52
1:A:27:GLY:O	1:A:28:LEU:HD22	2.10	0.52
1:A:206:TRP:O	1:A:243:PHE:HE1	1.93	0.52
1:A:32:PHE:C	1:A:32:PHE:CD1	2.81	0.51
1:A:61:VAL:HG12	1:A:309:ILE:CD1	2.29	0.51
1:A:40:LYS:CD	1:A:40:LYS:C	2.78	0.51
1:A:188:LEU:HD12	1:A:221:LEU:HG	1.92	0.51
1:A:228:GLY:HA3	1:A:233:LEU:HA	1.92	0.51
1:A:26:LEU:HD22	1:A:29:ALA:CB	2.24	0.51
1:A:393:THR:HG23	1:A:394:PRO:CG	2.41	0.51
1:A:204:GLU:HA	1:A:207:GLN:HB2	1.92	0.51
1:A:257:SER:HB3	1:A:263:TYR:CD2	2.45	0.51
1:A:309:ILE:HG21	1:A:319:TRP:CB	2.39	0.51
1:A:375:GLU:HG3	1:A:376:GLU:N	2.26	0.51
1:A:349:ASP:OD2	1:A:351:SER:OG	2.20	0.51
1:A:128:LYS:HZ1	1:A:129:ASN:CB	2.24	0.51
1:A:40:LYS:HD3	1:A:40:LYS:C	2.31	0.51
1:A:136:TRP:HB3	1:A:157:ARG:HB3	1.93	0.50
1:A:83:ILE:HD11	1:A:303:ALA:HB3	1.93	0.50
1:A:189:PHE:CE1	1:A:209:LEU:HD23	2.46	0.50
1:A:37:ARG:HB2	1:A:38:PRO:CD	2.29	0.50
1:A:84:PRO:HA	1:A:87:GLY:CA	2.39	0.50
1:A:165:GLU:O	1:A:167:HIS:ND1	2.44	0.50
1:A:174:LEU:HD22	1:A:178:LEU:HB2	1.93	0.50
1:A:404:ILE:CA	1:A:407:VAL:HG22	2.41	0.50
1:A:58:LEU:O	1:A:322:GLU:OE2	2.29	0.50
1:A:165:GLU:O	1:A:167:HIS:CG	2.64	0.50
1:A:332:ARG:HH21	1:A:336:LEU:HD21	1.76	0.50
1:A:375:GLU:HG3	1:A:377:PHE:N	2.26	0.50
1:A:327:ARG:O	1:A:328:GLN:C	2.49	0.50
1:A:404:ILE:C	1:A:407:VAL:HG22	2.31	0.50
1:A:274:ALA:HB3	1:A:280:VAL:HG12	1.94	0.50
1:A:276:ASP:C	1:A:278:GLU:N	2.65	0.50
1:A:70:GLU:HA	1:A:70:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASN:O	1:A:348:ARG:HB3	2.11	0.50
1:A:352:PHE:HB2	1:A:356:GLN:NE2	2.27	0.50
1:A:234:GLU:C	1:A:236:ASP:N	2.64	0.50
1:A:20:ALA:HB3	1:A:21:PRO:CD	2.30	0.50
1:A:276:ASP:CB	1:A:279:THR:H	2.20	0.50
1:A:145:HIS:CE1	1:A:188:LEU:HD21	2.47	0.49
1:A:43:LEU:O	1:A:380:TYR:O	2.29	0.49
1:A:282:ARG:O	1:A:285:SER:OG	2.20	0.49
1:A:140:PRO:HG2	1:A:196:PRO:HD2	1.94	0.49
1:A:135:VAL:O	1:A:157:ARG:N	2.44	0.49
1:A:349:ASP:C	1:A:351:SER:H	2.15	0.49
1:A:372:ARG:O	1:A:375:GLU:CB	2.58	0.49
1:A:175:ILE:HD13	1:A:209:LEU:HD12	1.93	0.49
1:A:179:ASN:HA	1:A:218:TRP:HZ2	1.76	0.49
1:A:107:ALA:HA	1:A:272:LEU:O	2.12	0.49
1:A:382:VAL:HG12	1:A:386:ARG:HB3	1.95	0.49
1:A:309:ILE:O	1:A:316:ARG:HG2	2.13	0.49
1:A:193:CYS:SG	1:A:200:ASP:CB	3.01	0.49
1:A:59:THR:CG2	1:A:322:GLU:OE1	2.61	0.49
1:A:57:VAL:HG11	1:A:62:LYS:HE2	1.95	0.49
1:A:137:VAL:O	1:A:138:SER:CB	2.60	0.49
1:A:183:ALA:O	1:A:185:ASP:N	2.46	0.48
1:A:210:ALA:O	1:A:213:SER:N	2.46	0.48
1:A:366:THR:O	1:A:368:GLU:HG2	2.12	0.48
1:A:334:ARG:HH12	1:A:361:SER:HB2	1.77	0.48
1:A:405:VAL:O	1:A:408:LEU:HA	2.13	0.48
1:A:272:LEU:HD23	1:A:280:VAL:HG23	1.94	0.48
1:A:179:ASN:HB2	1:A:216:LYS:HE2	1.94	0.48
1:A:97:LYS:HD2	1:A:98:GLY:H	1.78	0.48
1:A:231:ARG:NH1	1:A:235:GLU:CG	2.76	0.48
1:A:136:TRP:HZ2	1:A:181:ALA:H	1.59	0.48
1:A:45:ILE:HG22	1:A:47:VAL:N	2.24	0.48
1:A:94:LEU:O	1:A:237:ALA:HB1	2.14	0.48
1:A:213:SER:HA	1:A:218:TRP:HE3	1.78	0.48
1:A:370:VAL:CG1	1:A:381:ALA:HB3	2.44	0.48
1:A:40:LYS:C	1:A:40:LYS:NZ	2.60	0.48
1:A:220:PRO:CD	1:A:247:HIS:CE1	2.91	0.48
1:A:382:VAL:HG13	1:A:384:SER:OG	2.13	0.48
1:A:126:LEU:HG	1:A:130:THR:HG21	1.96	0.48
1:A:49:LYS:HG2	1:A:55:THR:HG23	1.96	0.48
1:A:287:MET:C	1:A:289:ALA:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:O	1:A:176:ASN:N	2.46	0.48
1:A:337:PHE:CD1	1:A:392:MET:HE1	2.48	0.48
1:A:119:LEU:HD13	1:A:145:HIS:CD2	2.49	0.48
1:A:178:LEU:HD23	1:A:218:TRP:CZ3	2.49	0.48
1:A:223:ASP:OD1	3:A:1:PMP:N1	2.47	0.48
1:A:14:PHE:O	1:A:14:PHE:CD1	2.67	0.48
1:A:146:LYS:HA	1:A:156:VAL:HG11	1.96	0.48
1:A:174:LEU:C	1:A:176:ASN:N	2.65	0.48
1:A:112:THR:HG22	1:A:269:ALA:CA	2.42	0.48
1:A:234:GLU:O	1:A:235:GLU:C	2.52	0.47
1:A:202:THR:H	1:A:205:GLN:CG	2.27	0.47
1:A:213:SER:HA	1:A:218:TRP:CE3	2.49	0.47
1:A:228:GLY:O	1:A:323:LEU:HD21	2.14	0.47
1:A:310:LEU:HA	1:A:316:ARG:HH11	1.79	0.47
1:A:232:GLY:HA2	1:A:327:ARG:NH1	2.30	0.47
1:A:393:THR:CB	1:A:394:PRO:HD2	2.42	0.47
1:A:305:VAL:O	1:A:305:VAL:HG13	2.14	0.47
1:A:37:ARG:CB	1:A:38:PRO:CD	2.91	0.47
1:A:392:MET:HG2	1:A:400:LEU:CD2	2.41	0.47
1:A:50:ASP:O	1:A:52:THR:N	2.37	0.47
1:A:194:HIS:HB3	1:A:197:THR:C	2.34	0.47
1:A:32:PHE:HA	1:A:380:TYR:CE2	2.50	0.47
1:A:393:THR:CG2	1:A:394:PRO:HD2	2.44	0.47
1:A:357:ASN:OD1	1:A:358:GLY:N	2.47	0.47
1:A:144:ASN:ND2	1:A:148:VAL:HG12	2.30	0.47
1:A:179:ASN:OD1	1:A:179:ASN:C	2.52	0.47
1:A:229:PHE:CE2	1:A:359:MET:CE	2.96	0.47
1:A:118:ALA:HA	1:A:121:VAL:CG1	2.45	0.47
1:A:167:HIS:H	1:A:167:HIS:CD2	2.32	0.47
1:A:203:LEU:C	1:A:207:GLN:HE21	2.19	0.47
1:A:360:PHE:O	1:A:361:SER:OG	2.31	0.47
1:A:192:CYS:SG	1:A:236:ASP:OD1	2.73	0.47
1:A:171:PHE:CZ	1:A:208:THR:HG21	2.50	0.47
1:A:75:LYS:O	1:A:75:LYS:HG3	2.14	0.47
1:A:100:ALA:O	1:A:104:ASP:HB2	2.15	0.47
1:A:86:PHE:O	1:A:90:THR:HB	2.15	0.47
1:A:321:GLN:NE2	1:A:325:ASP:CG	2.69	0.47
1:A:128:LYS:NZ	1:A:129:ASN:CB	2.78	0.46
1:A:26:LEU:HA	1:A:29:ALA:HB2	1.97	0.46
1:A:351:SER:O	1:A:352:PHE:C	2.53	0.46
1:A:174:LEU:CD1	1:A:209:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:TYR:HA	1:A:259:ASN:OD1	2.15	0.46
1:A:372:ARG:O	1:A:375:GLU:CG	2.62	0.46
1:A:105:LYS:O	1:A:106:ARG:HB3	2.15	0.46
1:A:45:ILE:CG2	1:A:47:VAL:N	2.68	0.46
1:A:231:ARG:CD	1:A:235:GLU:HG2	2.45	0.46
1:A:262:LEU:HD23	1:A:306:VAL:CG2	2.45	0.46
1:A:364:GLY:C	1:A:365:LEU:HD22	2.35	0.46
1:A:393:THR:HG23	1:A:394:PRO:HG2	1.96	0.46
1:A:293:ALA:O	1:A:294:ASN:O	2.33	0.46
1:A:174:LEU:O	1:A:175:ILE:C	2.54	0.46
1:A:348:ARG:NE	1:A:350:PHE:HE1	2.14	0.46
1:A:202:THR:N	1:A:205:GLN:HG3	2.30	0.46
1:A:188:LEU:HD12	1:A:221:LEU:HB3	1.98	0.46
1:A:256:TYR:HD2	1:A:260:PHE:CD2	2.34	0.46
1:A:342:GLN:O	1:A:342:GLN:CG	2.63	0.46
1:A:201:PRO:CB	1:A:205:GLN:HB2	2.46	0.46
1:A:40:LYS:CD	1:A:41:ILE:N	2.79	0.46
1:A:83:ILE:HA	1:A:84:PRO:HD3	1.81	0.46
1:A:377:PHE:HB3	1:A:379:VAL:HG13	1.98	0.46
1:A:142:TRP:CZ2	1:A:144:ASN:HB3	2.50	0.46
1:A:221:LEU:O	1:A:222:PHE:CB	2.55	0.46
1:A:99:SER:C	1:A:101:LEU:H	2.18	0.46
1:A:204:GLU:O	1:A:208:THR:N	2.49	0.45
1:A:32:PHE:CD1	1:A:32:PHE:O	2.70	0.45
1:A:334:ARG:HH22	1:A:360:PHE:C	2.19	0.45
1:A:352:PHE:O	1:A:356:GLN:HB3	2.16	0.45
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.81	0.45
1:A:76:ASN:O	1:A:77:TYR:C	2.54	0.45
1:A:312:ASN:O	1:A:316:ARG:CB	2.53	0.45
1:A:334:ARG:NH1	1:A:361:SER:OG	2.50	0.45
1:A:136:TRP:HA	1:A:157:ARG:H	1.81	0.45
1:A:208:THR:O	1:A:212:LEU:HD23	2.16	0.45
1:A:377:PHE:CZ	1:A:403:ALA:O	2.69	0.45
1:A:396:ASN:N	1:A:396:ASN:ND2	2.60	0.45
1:A:100:ALA:C	1:A:103:ASN:H	2.20	0.45
1:A:375:GLU:CG	1:A:376:GLU:H	2.30	0.45
1:A:86:PHE:CE2	1:A:269:ALA:HB2	2.40	0.45
1:A:78:LEU:HA	1:A:78:LEU:HD12	1.57	0.45
1:A:202:THR:N	1:A:205:GLN:NE2	2.22	0.45
1:A:70:GLU:CA	1:A:70:GLU:OE2	2.64	0.45
1:A:116:THR:CG2	1:A:142:TRP:CH2	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:TYR:C	1:A:265:GLU:N	2.66	0.45
1:A:374:ARG:HD3	1:A:374:ARG:HH11	1.44	0.45
1:A:140:PRO:HG2	1:A:140:PRO:O	2.16	0.45
1:A:199:ILE:O	1:A:200:ASP:CB	2.28	0.45
1:A:228:GLY:CA	1:A:233:LEU:HA	2.47	0.45
1:A:348:ARG:NH2	1:A:348:ARG:CG	2.69	0.45
1:A:398:ALA:HB3	1:A:399:PRO:HD2	1.99	0.45
1:A:111:GLN:NE2	1:A:303:ALA:CB	2.73	0.45
1:A:276:ASP:C	1:A:278:GLU:H	2.20	0.45
1:A:32:PHE:CD1	1:A:380:TYR:CE1	3.05	0.45
1:A:291:ILE:HG23	1:A:295:TYR:CE2	2.52	0.45
1:A:48:TYR:O	1:A:49:LYS:CB	2.65	0.44
1:A:291:ILE:CG2	1:A:295:TYR:CE2	2.99	0.44
1:A:204:GLU:CA	1:A:207:GLN:HB2	2.47	0.44
1:A:334:ARG:HG2	1:A:353:ILE:HG13	1.98	0.44
1:A:363:SER:HB2	1:A:365:LEU:HD21	2.00	0.44
1:A:388:ASN:C	1:A:390:ALA:N	2.71	0.44
1:A:206:TRP:CE3	1:A:206:TRP:HA	2.51	0.44
1:A:48:TYR:CE2	1:A:326:MET:HG3	2.51	0.44
1:A:50:ASP:HA	1:A:329:ARG:NH1	2.32	0.44
1:A:108:ARG:HH21	1:A:281:ASP:HA	1.82	0.44
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.69	0.44
1:A:43:LEU:HD23	1:A:387:VAL:CG2	2.47	0.44
1:A:100:ALA:O	1:A:103:ASN:C	2.56	0.44
1:A:274:ALA:HB3	1:A:280:VAL:CG1	2.48	0.44
1:A:136:TRP:CD2	1:A:157:ARG:HB3	2.53	0.44
1:A:337:PHE:HA	1:A:397:MET:HE1	1.99	0.44
1:A:247:HIS:HB3	1:A:248:LYS:H	1.26	0.44
1:A:255:SER:HA	1:A:268:GLY:HA3	1.98	0.44
1:A:393:THR:HB	1:A:396:ASN:ND2	2.32	0.44
1:A:212:LEU:O	1:A:213:SER:C	2.55	0.44
1:A:312:ASN:HB3	1:A:315:LEU:CB	2.48	0.44
1:A:178:LEU:HD21	1:A:218:TRP:CZ3	2.53	0.44
1:A:394:PRO:CG	1:A:395:ASP:N	2.81	0.44
1:A:404:ILE:CG2	1:A:405:VAL:N	2.80	0.44
1:A:108:ARG:NH2	1:A:281:ASP:OD2	2.45	0.44
1:A:398:ALA:O	1:A:401:CYS:HB3	2.18	0.44
1:A:112:THR:HA	1:A:113:PRO:HD3	1.80	0.44
1:A:91:GLN:HG3	1:A:102:ILE:HD11	1.99	0.44
1:A:28:LEU:HD12	1:A:380:TYR:HD2	1.83	0.43
1:A:229:PHE:CE2	1:A:359:MET:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:O	1:A:37:ARG:CB	2.54	0.43
1:A:396:ASN:H	1:A:396:ASN:ND2	2.13	0.43
1:A:179:ASN:CA	1:A:216:LYS:HE2	2.48	0.43
1:A:26:LEU:O	1:A:29:ALA:N	2.50	0.43
1:A:232:GLY:CA	1:A:327:ARG:NH1	2.81	0.43
1:A:335:GLN:N	1:A:354:ILE:HG23	2.32	0.43
1:A:367:LYS:O	1:A:370:VAL:HB	2.17	0.43
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.48	0.43
1:A:86:PHE:CD2	1:A:111:GLN:HG3	2.53	0.43
1:A:174:LEU:HD11	1:A:209:LEU:HD11	2.00	0.43
1:A:224:PHE:CE2	1:A:227:GLN:HG2	2.53	0.43
1:A:200:ASP:OD1	1:A:200:ASP:O	2.36	0.43
1:A:195:ASN:ND2	1:A:386:ARG:HD2	2.33	0.43
1:A:45:ILE:HG23	1:A:47:VAL:N	2.29	0.43
1:A:214:VAL:HG12	1:A:215:GLU:N	2.33	0.43
1:A:181:ALA:HB1	1:A:182:GLN:H	1.47	0.43
1:A:291:ILE:H	1:A:291:ILE:HG12	1.56	0.43
1:A:225:ALA:O	1:A:226:TYR:HB2	2.18	0.43
1:A:18:THR:HG22	1:A:19:ALA:H	1.84	0.43
1:A:210:ALA:HB2	1:A:243:PHE:CZ	2.54	0.43
1:A:202:THR:OG1	1:A:205:GLN:NE2	2.52	0.43
1:A:122:ALA:CB	1:A:251:ILE:HD11	2.48	0.43
1:A:99:SER:C	1:A:101:LEU:N	2.73	0.43
1:A:149:PHE:CE2	1:A:188:LEU:HD13	2.54	0.42
1:A:59:THR:O	1:A:60:SER:C	2.55	0.42
1:A:136:TRP:CH2	1:A:180:GLU:HB3	2.54	0.42
1:A:365:LEU:HA	1:A:369:GLN:CD	2.40	0.42
1:A:173:ALA:O	1:A:177:SER:N	2.51	0.42
1:A:337:PHE:HE2	1:A:350:PHE:HD2	1.66	0.42
1:A:122:ALA:HB1	1:A:251:ILE:HD11	2.01	0.42
1:A:149:PHE:HB3	1:A:156:VAL:HG12	2.00	0.42
1:A:329:ARG:HE	1:A:329:ARG:HB3	1.35	0.42
1:A:332:ARG:HG3	1:A:333:MET:N	2.33	0.42
1:A:367:LYS:HD3	1:A:368:GLU:CD	2.40	0.42
1:A:371:LEU:O	1:A:374:ARG:HB3	2.20	0.42
1:A:32:PHE:CD1	1:A:380:TYR:CD1	3.07	0.42
1:A:40:LYS:NZ	1:A:396:ASN:CB	2.82	0.42
1:A:47:VAL:O	1:A:48:TYR:O	2.38	0.42
1:A:91:GLN:HB3	1:A:92:GLU:H	1.53	0.42
1:A:252:VAL:HG13	1:A:271:THR:HG23	2.02	0.42
1:A:200:ASP:HA	1:A:201:PRO:HD3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:CE1	1:A:306:VAL:HG22	2.54	0.42
1:A:377:PHE:HB3	1:A:379:VAL:CG1	2.50	0.42
1:A:40:LYS:NZ	1:A:396:ASN:CG	2.67	0.42
1:A:379:VAL:HG11	1:A:403:ALA:CB	2.49	0.42
1:A:99:SER:O	1:A:102:ILE:HB	2.19	0.42
1:A:266:ARG:HG2	1:A:266:ARG:H	1.43	0.42
1:A:179:ASN:CB	1:A:216:LYS:HE2	2.50	0.42
1:A:334:ARG:HH12	1:A:361:SER:CB	2.32	0.42
1:A:76:ASN:C	1:A:77:TYR:O	2.57	0.42
1:A:59:THR:HG22	1:A:322:GLU:OE1	2.20	0.41
1:A:398:ALA:CB	1:A:399:PRO:CD	2.98	0.41
1:A:111:GLN:HB3	1:A:298:PRO:HG3	2.02	0.41
1:A:83:ILE:HD11	1:A:303:ALA:CB	2.50	0.41
1:A:321:GLN:O	1:A:321:GLN:NE2	2.47	0.41
1:A:116:THR:CG2	1:A:142:TRP:HH2	2.32	0.41
1:A:227:GLN:HE21	1:A:228:GLY:N	2.18	0.41
1:A:92:GLU:O	1:A:96:GLY:CA	2.67	0.41
1:A:48:TYR:CG	1:A:49:LYS:N	2.87	0.41
1:A:61:VAL:O	1:A:65:GLU:CG	2.68	0.41
1:A:188:LEU:HD12	1:A:221:LEU:CB	2.50	0.41
1:A:28:LEU:HD12	1:A:380:TYR:CD2	2.55	0.41
1:A:40:LYS:HE2	1:A:400:LEU:CB	2.51	0.41
1:A:85:GLU:HA	1:A:88:ARG:HG3	2.02	0.41
1:A:41:ILE:HA	1:A:41:ILE:HD12	1.72	0.41
1:A:182:GLN:O	1:A:183:ALA:C	2.58	0.41
1:A:337:PHE:CD1	1:A:392:MET:HE2	2.56	0.41
1:A:276:ASP:OD1	1:A:279:THR:OG1	2.39	0.41
1:A:136:TRP:HH2	1:A:180:GLU:CD	2.24	0.41
1:A:352:PHE:O	1:A:353:ILE:C	2.59	0.41
1:A:142:TRP:HA	1:A:143:PRO:HD3	1.84	0.41
1:A:327:ARG:O	1:A:329:ARG:N	2.54	0.41
1:A:356:GLN:OE1	1:A:361:SER:CB	2.69	0.41
1:A:78:LEU:HD22	1:A:300:ALA:CB	2.49	0.41
1:A:108:ARG:NH2	1:A:281:ASP:HA	2.36	0.41
1:A:197:THR:C	1:A:199:ILE:N	2.72	0.40
1:A:351:SER:O	1:A:354:ILE:N	2.54	0.40
1:A:32:PHE:HB2	1:A:380:TYR:CD2	2.55	0.40
1:A:350:PHE:HA	1:A:352:PHE:HE1	1.85	0.40
1:A:350:PHE:HA	1:A:352:PHE:CE1	2.56	0.40
1:A:404:ILE:HG23	1:A:405:VAL:N	2.36	0.40
1:A:51:GLU:HG3	1:A:329:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:C	1:A:159:TYR:O	2.59	0.40
1:A:231:ARG:NH2	1:A:357:ASN:ND2	2.70	0.40
1:A:276:ASP:HB2	1:A:279:THR:CB	2.51	0.40
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.84	0.40
1:A:223:ASP:OD1	3:A:1:PMP:H2A2	2.21	0.40
1:A:226:TYR:O	1:A:227:GLN:C	2.59	0.40
1:A:118:ALA:HA	1:A:121:VAL:HG12	2.04	0.40
1:A:250:LEU:HD12	1:A:273:VAL:HG11	2.03	0.40
1:A:212:LEU:N	1:A:212:LEU:CD2	2.84	0.40
1:A:333:MET:CE	1:A:392:MET:HB3	2.51	0.40
1:A:40:LYS:HD2	1:A:43:LEU:HD13	2.02	0.40
1:A:43:LEU:O	1:A:381:ALA:HA	2.22	0.40
1:A:17:ILE:HG23	1:A:17:ILE:O	2.21	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PHE:CZ	1:A:273:VAL:O[4_566]	1.53	0.67
1:A:55:THR:O	1:A:74:THR:OG1[4_566]	1.61	0.59
1:A:264:ASN:OD1	1:A:300:ALA:CB[4_566]	1.79	0.41
1:A:264:ASN:O	1:A:298:PRO:O[4_566]	1.82	0.38
1:A:120:ARG:NE	1:A:294:ASN:ND2[4_566]	1.91	0.29
1:A:165:GLU:OE2	1:A:282:ARG:NH1[7_645]	1.92	0.28
1:A:116:THR:CG2	1:A:296:SER:OG[4_566]	1.98	0.22
1:A:15:GLU:OE1	1:A:274:ALA:CB[4_566]	2.03	0.17
1:A:13:MET:CB	1:A:366:THR:OG1[6_655]	2.08	0.12
1:A:18:THR:OG1	1:A:129:ASN:ND2[4_566]	2.12	0.08
1:A:120:ARG:CD	1:A:294:ASN:ND2[4_566]	2.15	0.05
1:A:15:GLU:OE2	1:A:249:GLU:CG[4_566]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	394/396 (100%)	249 (63%)	75 (19%)	70 (18%)	0 0

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA
1	A	22	ALA
1	A	27	GLY
1	A	34	ALA
1	A	40	LYS
1	A	41	ILE
1	A	48	TYR
1	A	58	LEU
1	A	59	THR
1	A	60	SER
1	A	73	THR
1	A	75	LYS
1	A	97	LYS
1	A	114	GLY
1	A	129	ASN
1	A	138	SER
1	A	160	ALA
1	A	199	ILE
1	A	200	ASP
1	A	214	VAL
1	A	218	TRP
1	A	222	PHE
1	A	247	HIS
1	A	248	LYS
1	A	258	ALA
1	A	263	TYR
1	A	294	ASN
1	A	300	ALA
1	A	357	ASN
1	A	367	LYS
1	A	375	GLU
1	A	398	ALA
1	A	17	ILE
1	A	29	ALA
1	A	31	LEU
1	A	49	LYS

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Mol	Chain	Res	Type
1	A	115	GLY
1	A	128	LYS
1	A	153	GLY
1	A	180	GLU
1	A	183	ALA
1	A	184	GLY
1	A	191	GLY
1	A	194	HIS
1	A	198	GLY
1	A	233	LEU
1	A	264	ASN
1	A	328	GLN
1	A	344	LYS
1	A	345	GLY
1	A	356	GLN
1	A	368	GLU
1	A	397	MET
1	A	38	PRO
1	A	51	GLU
1	A	74	THR
1	A	159	TYR
1	A	164	ALA
1	A	227	GLN
1	A	297	ASN
1	A	346	ALA
1	A	352	PHE
1	A	77	TYR
1	A	154	LEU
1	A	219	LEU
1	A	80	ILE
1	A	235	GLU
1	A	266	ARG
1	A	366	THR
1	A	44	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	319/319 (100%)	166 (52%)	153 (48%)	0 0

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	14	PHE
1	A	15	GLU
1	A	17	ILE
1	A	24	PRO
1	A	25	ILE
1	A	26	LEU
1	A	28	LEU
1	A	31	LEU
1	A	33	ARG
1	A	35	ASP
1	A	36	GLU
1	A	40	LYS
1	A	41	ILE
1	A	43	LEU
1	A	45	ILE
1	A	47	VAL
1	A	51	GLU
1	A	54	LYS
1	A	55	THR
1	A	61	VAL
1	A	62	LYS
1	A	66	GLN
1	A	71	ASN
1	A	74	THR
1	A	75	LYS
1	A	76	ASN
1	A	80	ILE
1	A	81	ASP
1	A	83	ILE
1	A	88	ARG
1	A	89	CYS
1	A	90	THR
1	A	93	LEU
1	A	97	LYS
1	A	101	LEU
1	A	103	ASN
1	A	104	ASP

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Mol	Chain	Res	Type
1	A	109	THR
1	A	112	THR
1	A	116	THR
1	A	124	ASP
1	A	125	PHE
1	A	128	LYS
1	A	132	VAL
1	A	134	ARG
1	A	135	VAL
1	A	136	TRP
1	A	144	ASN
1	A	145	HIS
1	A	146	LYS
1	A	148	VAL
1	A	149	PHE
1	A	154	LEU
1	A	157	ARG
1	A	159	TYR
1	A	161	TYR
1	A	166	ASN
1	A	170	ASP
1	A	171	PHE
1	A	172	ASP
1	A	174	LEU
1	A	177	SER
1	A	179	ASN
1	A	182	GLN
1	A	185	ASP
1	A	186	VAL
1	A	189	PHE
1	A	190	HIS
1	A	192	CYS
1	A	193	CYS
1	A	195	ASN
1	A	200	ASP
1	A	203	LEU
1	A	204	GLU
1	A	206	TRP
1	A	207	GLN
1	A	211	GLN
1	A	212	LEU
1	A	213	SER

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Mol	Chain	Res	Type
1	A	215	GLU
1	A	219	LEU
1	A	221	LEU
1	A	224	PHE
1	A	227	GLN
1	A	235	GLU
1	A	236	ASP
1	A	240	LEU
1	A	241	ARG
1	A	243	PHE
1	A	246	MET
1	A	247	HIS
1	A	248	LYS
1	A	250	LEU
1	A	251	ILE
1	A	252	VAL
1	A	254	SER
1	A	255	SER
1	A	259	ASN
1	A	260	PHE
1	A	262	LEU
1	A	263	TYR
1	A	265	GLU
1	A	266	ARG
1	A	271	THR
1	A	273	VAL
1	A	277	SER
1	A	280	VAL
1	A	282	ARG
1	A	286	GLN
1	A	291	ILE
1	A	296	SER
1	A	305	VAL
1	A	310	LEU
1	A	312	ASN
1	A	313	ASP
1	A	315	LEU
1	A	316	ARG
1	A	321	GLN
1	A	322	GLU
1	A	326	MET
1	A	327	ARG

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Mol	Chain	Res	Type
1	A	328	GLN
1	A	329	ARG
1	A	330	ILE
1	A	332	ARG
1	A	334	ARG
1	A	336	LEU
1	A	339	ASN
1	A	347	ASN
1	A	348	ARG
1	A	353	ILE
1	A	354	ILE
1	A	356	GLN
1	A	357	ASN
1	A	362	PHE
1	A	365	LEU
1	A	367	LYS
1	A	369	GLN
1	A	372	ARG
1	A	373	LEU
1	A	374	ARG
1	A	375	GLU
1	A	376	GLU
1	A	379	VAL
1	A	382	VAL
1	A	387	VAL
1	A	396	ASN
1	A	397	MET
1	A	400	LEU
1	A	402	GLU
1	A	404	ILE
1	A	408	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	111	GLN
1	A	144	ASN
1	A	166	ASN
1	A	167	HIS
1	A	190	HIS
1	A	195	ASN

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Mol	Chain	Res	Type
1	A	205	GLN
1	A	207	GLN
1	A	227	GLN
1	A	294	ASN
1	A	312	ASN
1	A	321	GLN
1	A	331	GLN
1	A	339	ASN
1	A	388	ASN

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PMP	A	1	-	16,16,16	1.18	3 (18%)	20,23,23	2.50	9 (45%)
2	SO4	A	2	-	4,4,4	1.11	0	6,6,6	1.08	0

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	PMP	A	1	-	-	0/8/8/8	0/1/1/1
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	PMP	C5-C4	-2.36	1.37	1.40
3	A	1	PMP	O3-C3	-2.28	1.31	1.37
3	A	1	PMP	C4A-C4	-2.06	1.44	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	PMP	C3-C2-N1	-3.39	115.92	120.61
3	A	1	PMP	C5-C6-N1	-3.16	118.38	123.86
3	A	1	PMP	C5A-C5-C6	-2.10	115.31	119.28
3	A	1	PMP	O3P-P-O4P	2.11	112.63	106.56
3	A	1	PMP	C5A-C5-C4	2.53	126.77	121.89
3	A	1	PMP	C3-C4-C5	2.71	121.67	118.82
3	A	1	PMP	C6-N1-C2	3.61	126.65	119.28
3	A	1	PMP	O4P-C5A-C5	4.45	116.35	108.99
3	A	1	PMP	O2P-P-O1P	5.36	127.84	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	PMP	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.