



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:46 AM GMT

PDB ID : 3G05
Title : Crystal structure of N-terminal domain (2-550) of E.coli MnmG
Authors : Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2009-01-27
Resolution : 3.49 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

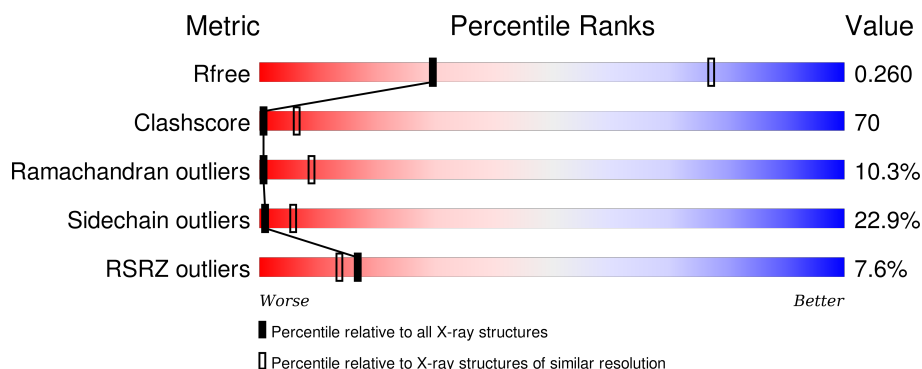
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	 5% 25% 48% 16% • 9%
1	B	576	 9% 21% 48% 19% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8156 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4073	2551	728	776	18			
1	B	524	Total	C	N	O	S	0	0	0
			4063	2540	730	775	18			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	EXPRESSION TAG	UNP Q8XAY0
A	-26	GLY	-	EXPRESSION TAG	UNP Q8XAY0
A	-25	SER	-	EXPRESSION TAG	UNP Q8XAY0
A	-24	SER	-	EXPRESSION TAG	UNP Q8XAY0
A	-23	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-22	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-21	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-20	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-19	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-18	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-17	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-16	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-15	ASP	-	EXPRESSION TAG	UNP Q8XAY0
A	-14	TYR	-	EXPRESSION TAG	UNP Q8XAY0
A	-13	ASP	-	EXPRESSION TAG	UNP Q8XAY0
A	-12	ILE	-	EXPRESSION TAG	UNP Q8XAY0
A	-11	PRO	-	EXPRESSION TAG	UNP Q8XAY0
A	-10	THR	-	EXPRESSION TAG	UNP Q8XAY0
A	-9	THR	-	EXPRESSION TAG	UNP Q8XAY0
A	-8	GLU	-	EXPRESSION TAG	UNP Q8XAY0
A	-7	ASN	-	EXPRESSION TAG	UNP Q8XAY0
A	-6	LEU	-	EXPRESSION TAG	UNP Q8XAY0
A	-5	TYR	-	EXPRESSION TAG	UNP Q8XAY0
A	-4	PHE	-	EXPRESSION TAG	UNP Q8XAY0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLN	-	EXPRESSION TAG	UNP Q8XAY0
A	-2	GLY	-	EXPRESSION TAG	UNP Q8XAY0
A	-1	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-27	MET	-	EXPRESSION TAG	UNP Q8XAY0
B	-26	GLY	-	EXPRESSION TAG	UNP Q8XAY0
B	-25	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-24	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-23	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-22	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-21	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-20	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-19	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-18	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-17	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-16	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-15	ASP	-	EXPRESSION TAG	UNP Q8XAY0
B	-14	TYR	-	EXPRESSION TAG	UNP Q8XAY0
B	-13	ASP	-	EXPRESSION TAG	UNP Q8XAY0
B	-12	ILE	-	EXPRESSION TAG	UNP Q8XAY0
B	-11	PRO	-	EXPRESSION TAG	UNP Q8XAY0
B	-10	THR	-	EXPRESSION TAG	UNP Q8XAY0
B	-9	THR	-	EXPRESSION TAG	UNP Q8XAY0
B	-8	GLU	-	EXPRESSION TAG	UNP Q8XAY0
B	-7	ASN	-	EXPRESSION TAG	UNP Q8XAY0
B	-6	LEU	-	EXPRESSION TAG	UNP Q8XAY0
B	-5	TYR	-	EXPRESSION TAG	UNP Q8XAY0
B	-4	PHE	-	EXPRESSION TAG	UNP Q8XAY0
B	-3	GLN	-	EXPRESSION TAG	UNP Q8XAY0
B	-2	GLY	-	EXPRESSION TAG	UNP Q8XAY0
B	-1	SER	-	EXPRESSION TAG	UNP Q8XAY0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

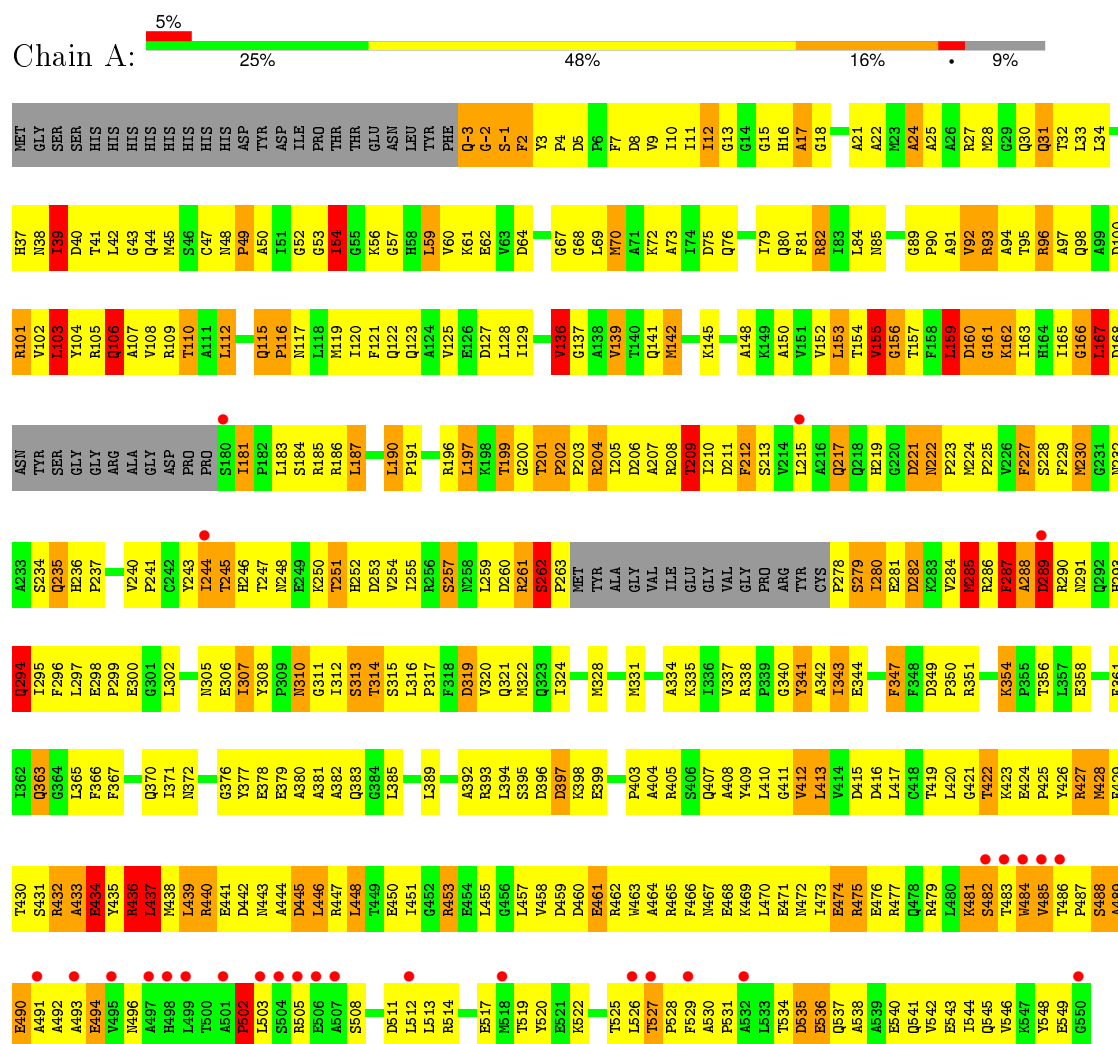


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

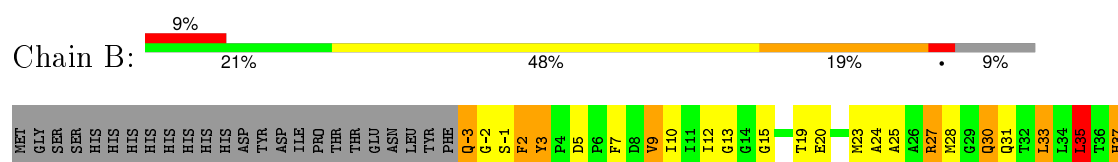
3 Residue-property plots

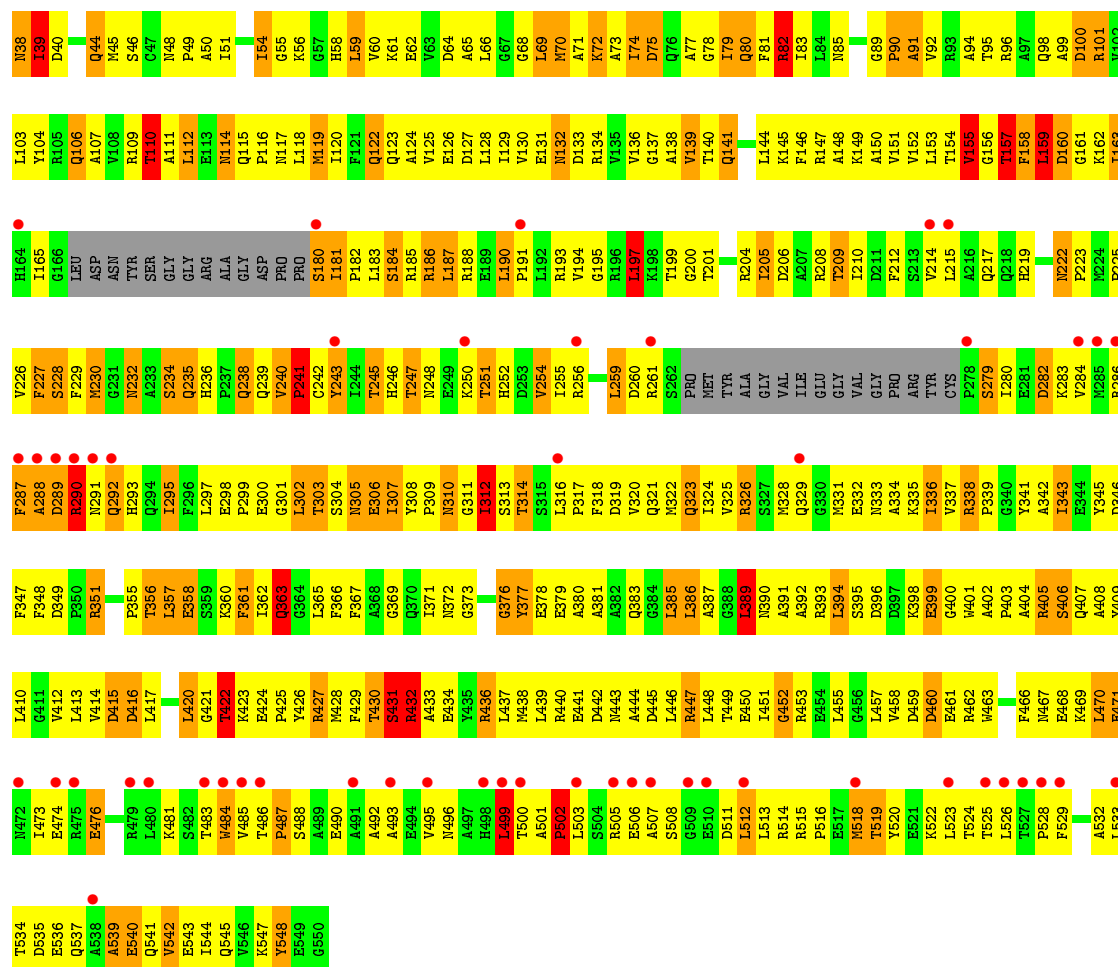
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG



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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.59Å 144.59Å 271.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.49 49.74 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.49) 99.7 (49.74-3.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.227 , 0.265 0.224 , 0.260	Depositor DCC
R_{free} test set	2137 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	91.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 83.0	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42342 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8156	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.84	1/4146 (0.0%)	1.15	20/5615 (0.4%)
1	B	0.75	0/4134	1.11	15/5596 (0.3%)
All	All	0.80	1/8280 (0.0%)	1.13	35/11211 (0.3%)

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	1	7
1	B	0	4
All	All	1	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	ARG	CZ-NH2	24.30	1.64	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	B	290	ARG	N-CA-C	-10.74	82.01	111.00
1	A	505	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	B	100	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	505	ARG	NH1-CZ-NH2	-7.68	110.95	119.40
1	B	101	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	B	112	LEU	CB-CG-CD2	-6.81	99.43	111.00
1	B	385	LEU	CA-CB-CG	-6.75	99.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	THR	CB-CA-C	-6.61	93.74	111.60
1	A	112	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	A	202	PRO	C-N-CD	6.54	142.14	128.40
1	B	402	ALA	C-N-CD	6.41	141.85	128.40
1	A	434	GLU	CB-CA-C	6.38	123.16	110.40
1	B	35	LEU	CA-CB-CG	6.33	129.86	115.30
1	A	103	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	A	314	THR	CB-CA-C	-6.18	94.91	111.60
1	A	197	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	204	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	416	ASP	CB-CG-OD1	-5.94	112.96	118.30
1	A	47	CYS	CA-CB-SG	-5.88	103.42	114.00
1	B	152	VAL	CB-CA-C	-5.78	100.42	111.40
1	A	427	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	75	ASP	CB-CG-OD1	-5.66	113.20	118.30
1	B	376	GLY	N-CA-C	5.54	126.95	113.10
1	A	446	LEU	CA-CB-CG	-5.44	102.78	115.30
1	A	59	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	B	159	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	103	LEU	CA-CB-CG	-5.29	103.13	115.30
1	B	112	LEU	CA-CB-CG	-5.19	103.36	115.30
1	A	197	LEU	N-CA-C	-5.16	97.06	111.00
1	A	101	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	197	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	505	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	436	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	B	155	VAL	CB-CA-C	-5.00	101.90	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	291	ASN	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	SER	Mainchain,Peptide
1	A	159	LEU	Peptide
1	A	261	ARG	Peptide
1	A	287	PHE	Peptide
1	A	288	ALA	Peptide
1	A	289	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	159	LEU	Peptide
1	B	241	PRO	Peptide
1	B	436	ARG	Peptide
1	B	89	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4073	0	4026	563	0
1	B	4063	0	4029	581	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
All	All	8156	0	8055	1141	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 70.

All (1141) 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:289:ASP:CA	1:A:291:ASN:HA	1.56	1.32
1:B:180:SER:O	1:B:181:ILE:HG22	1.24	1.31
1:B:154:THR:O	1:B:155:VAL:CG1	1.79	1.29
1:A:285:MET:CE	1:A:285:MET:HA	1.59	1.26
1:A:289:ASP:C	1:A:291:ASN:HA	1.56	1.26
1:A:432:ARG:HB2	1:A:436:ARG:NH1	1.52	1.25
1:A:285:MET:CA	1:A:285:MET:HE2	1.67	1.23
1:A:404:ALA:HB3	1:A:407:GLN:CG	1.68	1.23
1:B:12:ILE:O	1:B:154:THR:CG2	1.86	1.22
1:A:204:ARG:NH1	1:A:300:GLU:OE1	1.76	1.18
1:B:139:VAL:HG13	1:B:145:LYS:HG2	1.27	1.17
1:A:156:GLY:O	1:A:157:THR:HG22	1.43	1.16
1:B:154:THR:CG2	1:B:155:VAL:H	1.59	1.15
1:A:13:GLY:O	1:A:154:THR:HG21	1.47	1.15
1:A:262:SER:CB	1:A:263:PRO:HD2	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG21	1:A:328:MET:HE1	1.29	1.14
1:B:12:ILE:O	1:B:154:THR:HG22	0.97	1.14
1:A:314:THR:HG22	1:A:316:LEU:H	1.05	1.14
1:A:404:ALA:HB3	1:A:407:GLN:HG3	1.15	1.13
1:A:209:THR:CG2	1:A:335:LYS:HG3	1.79	1.13
1:A:209:THR:HG21	1:A:335:LYS:CG	1.79	1.12
1:A:314:THR:HG21	1:A:316:LEU:HB2	1.21	1.12
1:B:191:PRO:HB2	1:B:361:PHE:HE1	1.15	1.11
1:B:90:PRO:HB2	1:B:440:ARG:HD2	1.32	1.11
1:A:439:LEU:HD23	1:A:439:LEU:N	1.56	1.11
1:A:448:LEU:HD23	1:A:451:ILE:HD11	1.29	1.10
1:A:163:ILE:HG23	1:A:341:TYR:HD2	1.10	1.10
1:B:154:THR:HG23	1:B:155:VAL:H	0.94	1.09
1:A:285:MET:CA	1:A:285:MET:CE	2.25	1.08
1:A:284:VAL:O	1:A:286:ARG:N	1.85	1.08
1:A:-3:GLN:HG3	1:A:-3:GLN:O	1.46	1.08
1:A:290:ARG:N	1:A:291:ASN:HA	1.62	1.08
1:B:191:PRO:HB2	1:B:361:PHE:CE1	1.89	1.07
1:B:209:THR:OG1	1:B:334:ALA:HA	1.55	1.07
1:A:209:THR:HB	1:A:334:ALA:HA	1.36	1.07
1:B:401:TRP:CZ2	1:B:403:PRO:HB3	1.89	1.07
1:A:404:ALA:CB	1:A:407:GLN:HG3	1.84	1.06
1:A:262:SER:CB	1:A:263:PRO:CD	2.32	1.06
1:B:461:GLU:HG2	1:B:461:GLU:O	1.54	1.06
1:B:230:MET:HE3	1:B:230:MET:HA	1.31	1.06
1:A:289:ASP:CA	1:A:291:ASN:CA	2.33	1.06
1:B:347:PHE:HB2	1:B:371:ILE:O	1.55	1.06
1:B:154:THR:O	1:B:155:VAL:HG12	0.89	1.05
1:B:81:PHE:CE2	1:B:236:HIS:CD2	2.43	1.05
1:A:250:LYS:O	1:A:254:VAL:HG23	1.57	1.05
1:A:440:ARG:HH21	1:A:544:ILE:HG21	1.17	1.04
1:B:154:THR:C	1:B:155:VAL:HG12	1.75	1.04
1:B:154:THR:HG23	1:B:155:VAL:N	1.64	1.04
1:A:314:THR:HG22	1:A:315:SER:N	1.74	1.03
1:A:351:ARG:HD2	1:A:421:GLY:CA	1.88	1.03
1:A:314:THR:HG22	1:A:315:SER:H	1.23	1.03
1:A:45:MET:CE	1:A:49:PRO:HA	1.89	1.03
1:B:45:MET:HG2	1:B:377:TYR:CE2	1.94	1.02
1:B:180:SER:O	1:B:181:ILE:CG2	2.07	1.02
1:B:156:GLY:O	1:B:157:THR:HG23	1.57	1.02
1:A:166:GLY:N	1:A:315:SER:O	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HG21	1:A:210:ILE:HD11	1.42	1.01
1:B:230:MET:CE	1:B:230:MET:HA	1.89	1.01
1:A:262:SER:OG	1:A:263:PRO:HD2	1.57	1.01
1:B:252:HIS:HD2	1:B:284:VAL:HG11	1.26	1.01
1:B:155:VAL:HG22	1:B:155:VAL:O	1.56	1.01
1:A:159:LEU:HB3	1:A:160:ASP:HA	1.42	1.00
1:B:210:ILE:HG22	1:B:212:PHE:CD2	1.97	1.00
1:B:209:THR:HG1	1:B:334:ALA:HA	1.19	0.99
1:B:205:ILE:CD1	1:B:336:ILE:HA	1.92	0.99
1:A:81:PHE:HB3	1:A:225:PRO:HG2	1.43	0.99
1:A:163:ILE:CG2	1:A:341:TYR:HD2	1.75	0.98
1:A:448:LEU:CD2	1:A:451:ILE:HD11	1.92	0.98
1:A:108:VAL:O	1:A:112:LEU:HD12	1.63	0.98
1:B:33:LEU:HD21	1:B:35:LEU:HD23	1.43	0.98
1:A:154:THR:O	1:A:155:VAL:HG12	1.62	0.97
1:A:45:MET:HE2	1:A:49:PRO:HA	1.44	0.97
1:A:448:LEU:O	1:A:451:ILE:HG12	1.63	0.97
1:A:163:ILE:HG23	1:A:341:TYR:CD2	1.98	0.96
1:B:394:LEU:HD23	1:B:394:LEU:C	1.83	0.96
1:A:289:ASP:N	1:A:291:ASN:CB	2.28	0.96
1:A:424:GLU:CD	1:A:436:ARG:HH22	1.67	0.96
1:A:166:GLY:HA3	1:A:317:PRO:HG3	1.48	0.96
1:B:191:PRO:CB	1:B:361:PHE:HE1	1.78	0.96
1:B:33:LEU:HD21	1:B:35:LEU:CD2	1.94	0.96
1:B:48:ASN:HB3	1:B:308:TYR:CE2	1.99	0.96
1:B:13:GLY:HA3	1:B:154:THR:CG2	1.96	0.96
1:A:338:ARG:HH21	1:B:39:ILE:HB	1.30	0.95
1:A:443:ASN:OD1	1:A:447:ARG:HD3	1.66	0.95
1:A:314:THR:HG22	1:A:316:LEU:N	1.80	0.95
1:A:285:MET:CE	1:A:285:MET:N	2.29	0.94
1:B:78:GLY:HA2	1:B:98:GLN:O	1.67	0.94
1:B:90:PRO:O	1:B:92:VAL:N	2.00	0.94
1:B:250:LYS:O	1:B:254:VAL:HG23	1.67	0.94
1:A:424:GLU:OE2	1:A:436:ARG:NH2	2.01	0.94
1:A:247:THR:HG22	1:A:293:HIS:H	1.29	0.94
1:A:289:ASP:N	1:A:291:ASN:HA	1.83	0.93
1:B:13:GLY:HA3	1:B:154:THR:HG21	1.47	0.93
1:B:314:THR:HG23	1:B:316:LEU:HB2	1.49	0.92
1:B:431:SER:O	1:B:433:ALA:N	2.00	0.92
1:B:31:GLN:HA	1:B:31:GLN:NE2	1.81	0.92
1:A:155:VAL:CG1	1:A:156:GLY:N	2.29	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:O	1:A:213:SER:N	2.03	0.92
1:B:139:VAL:HG13	1:B:145:LYS:CG	1.99	0.92
1:B:314:THR:CG2	1:B:316:LEU:HB2	1.99	0.92
1:B:210:ILE:CG2	1:B:212:PHE:CE2	2.51	0.92
1:A:439:LEU:N	1:A:439:LEU:CD2	2.33	0.92
1:A:314:THR:CG2	1:A:316:LEU:HB2	2.01	0.91
1:A:285:MET:HA	1:A:285:MET:HE2	0.93	0.91
1:A:437:LEU:HD12	1:A:437:LEU:O	1.70	0.91
1:A:203:PRO:HB3	1:A:340:GLY:H	1.34	0.91
1:A:155:VAL:HG13	1:A:156:GLY:N	1.86	0.90
1:A:320:VAL:O	1:A:324:ILE:HG13	1.71	0.90
1:A:101:ARG:NH1	1:A:300:GLU:OE2	2.04	0.90
1:A:285:MET:HE3	1:A:285:MET:N	1.86	0.90
1:B:217:GLN:NE2	1:B:219:HIS:NE2	2.20	0.90
1:B:79:ILE:HA	1:B:239:GLN:NE2	1.86	0.90
1:B:210:ILE:CG2	1:B:212:PHE:HE2	1.84	0.89
1:A:347:PHE:CG	1:A:347:PHE:O	2.25	0.89
1:B:160:ASP:CG	1:B:161:GLY:H	1.73	0.89
1:A:314:THR:CG2	1:A:316:LEU:H	1.86	0.89
1:B:101:ARG:HH12	1:B:300:GLU:CD	1.75	0.89
1:B:321:GLN:O	1:B:325:VAL:HG23	1.72	0.89
1:B:427:ARG:HH21	1:B:428:MET:HE1	1.37	0.89
1:A:530:ALA:HB1	1:A:531:PRO:HA	1.54	0.89
1:B:252:HIS:HD2	1:B:284:VAL:CG1	1.86	0.89
1:B:386:LEU:HD12	1:B:389:LEU:HD23	1.54	0.88
1:A:289:ASP:HA	1:A:291:ASN:CA	2.02	0.88
1:B:2:PHE:O	1:B:3:TYR:C	2.11	0.88
1:A:432:ARG:CB	1:A:436:ARG:NH1	2.34	0.88
1:A:351:ARG:HD2	1:A:421:GLY:N	1.89	0.86
1:A:289:ASP:C	1:A:291:ASN:CA	2.44	0.86
1:A:8:ASP:OD2	1:A:31:GLN:N	2.08	0.86
1:A:156:GLY:HA3	2:A:551:SO4:O4	1.74	0.86
1:B:201:THR:HG22	1:B:341:TYR:O	1.75	0.86
1:B:79:ILE:O	1:B:80:GLN:HB3	1.71	0.86
1:B:45:MET:HE3	1:B:104:TYR:CD1	2.10	0.86
1:B:469:LYS:O	1:B:473:ILE:HG13	1.76	0.86
1:B:518:MET:SD	1:B:523:LEU:HB2	2.15	0.86
1:B:127:ASP:HA	1:B:183:LEU:HB2	1.56	0.86
1:B:3:TYR:HD2	1:B:5:ASP:H	1.22	0.86
1:B:417:LEU:O	1:B:421:GLY:HA2	1.74	0.86
1:B:158:PHE:O	1:B:159:LEU:C	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PHE:N	1:B:361:PHE:CD2	2.40	0.85
1:A:288:ALA:O	1:A:291:ASN:CB	2.25	0.85
1:B:81:PHE:HB3	1:B:225:PRO:HG2	1.58	0.84
1:B:222:ASN:HD22	1:B:223:PRO:HA	1.40	0.84
1:A:284:VAL:C	1:A:286:ARG:H	1.79	0.84
1:B:476:GLU:HG3	1:B:476:GLU:O	1.75	0.84
1:A:139:VAL:HG13	1:A:145:LYS:HG2	1.58	0.84
1:A:122:GLN:HG2	1:A:122:GLN:O	1.75	0.84
1:B:361:PHE:N	1:B:361:PHE:HD2	1.71	0.84
1:A:163:ILE:CG2	1:A:341:TYR:CD2	2.59	0.84
1:B:181:ILE:HG23	1:B:184:SER:HB2	1.58	0.84
1:A:440:ARG:HH21	1:A:544:ILE:CG2	1.90	0.84
1:A:351:ARG:HD2	1:A:421:GLY:HA3	1.60	0.84
1:A:262:SER:HB2	1:A:263:PRO:HD2	1.57	0.84
1:A:253:ASP:O	1:A:257:SER:OG	1.95	0.84
1:B:314:THR:HG23	1:B:316:LEU:H	1.42	0.83
1:B:282:ASP:O	1:B:284:VAL:N	2.11	0.83
1:B:256:ARG:HA	1:B:259:LEU:HD12	1.59	0.83
1:B:38:ASN:O	1:B:40:ASP:N	2.12	0.83
1:A:436:ARG:O	1:A:437:LEU:HB2	1.79	0.83
1:B:314:THR:HG23	1:B:316:LEU:N	1.94	0.83
1:A:290:ARG:N	1:A:291:ASN:CA	2.36	0.83
1:A:262:SER:OG	1:A:263:PRO:CD	2.25	0.83
1:B:205:ILE:HD11	1:B:336:ILE:HA	1.60	0.83
1:A:81:PHE:CB	1:A:225:PRO:HG2	2.07	0.83
1:A:289:ASP:HA	1:A:291:ASN:CB	2.10	0.82
1:A:201:THR:HG22	1:A:202:PRO:HD2	1.61	0.82
1:B:13:GLY:CA	1:B:154:THR:HG21	2.10	0.82
1:B:210:ILE:HG22	1:B:212:PHE:CE2	2.13	0.82
1:B:226:VAL:HG21	1:B:232:ASN:HA	1.62	0.82
1:A:289:ASP:CA	1:A:291:ASN:CB	2.58	0.81
1:B:541:GLN:HG3	1:B:545:GLN:HE21	1.45	0.81
1:A:440:ARG:NH2	1:A:544:ILE:HG21	1.94	0.81
1:A:159:LEU:HB3	1:A:160:ASP:CA	2.09	0.81
1:B:427:ARG:HH21	1:B:428:MET:CE	1.93	0.81
1:B:81:PHE:CE2	1:B:236:HIS:HD2	1.93	0.81
1:B:96:ARG:HG2	1:B:96:ARG:O	1.78	0.81
1:B:540:GLU:O	1:B:544:ILE:HG12	1.80	0.81
1:B:366:PHE:CE1	1:B:391:ALA:HB2	2.15	0.81
1:B:453:ARG:NH2	1:B:460:ASP:OD1	2.13	0.81
1:A:432:ARG:HB2	1:A:436:ARG:HH11	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:SER:O	1:A:236:HIS:N	2.14	0.81
1:B:210:ILE:HG22	1:B:212:PHE:HD2	1.44	0.80
1:A:527:THR:N	1:A:528:PRO:HD2	1.96	0.80
1:A:453:ARG:HG2	1:A:463:TRP:CE2	2.16	0.80
1:B:100:ASP:HB3	1:B:103:LEU:HB2	1.63	0.80
1:A:154:THR:O	1:A:155:VAL:CG1	2.29	0.80
1:B:37:HIS:C	1:B:37:HIS:ND1	2.36	0.80
1:B:94:ALA:HA	1:B:441:GLU:OE2	1.82	0.79
1:A:289:ASP:N	1:A:291:ASN:CA	2.44	0.79
1:B:156:GLY:O	1:B:157:THR:CG2	2.29	0.79
1:A:372:ASN:HD22	1:A:383:GLN:HE21	1.31	0.78
1:B:541:GLN:HG3	1:B:545:GLN:NE2	1.97	0.78
1:A:382:ALA:HB1	1:A:410:LEU:HD23	1.64	0.78
1:B:210:ILE:HG21	1:B:212:PHE:HE2	1.49	0.78
1:B:79:ILE:O	1:B:80:GLN:CB	2.33	0.77
1:B:209:THR:HG21	1:B:335:LYS:HB2	1.66	0.77
1:B:158:PHE:O	1:B:158:PHE:CG	2.37	0.77
1:B:191:PRO:CG	1:B:361:PHE:CE1	2.67	0.77
1:A:49:PRO:HB3	1:A:101:ARG:NH1	1.99	0.77
1:B:73:ALA:HB1	1:B:104:TYR:CE2	2.18	0.77
1:B:33:LEU:CD2	1:B:35:LEU:HD23	2.15	0.77
1:A:205:ILE:CG2	1:A:210:ILE:HD11	2.14	0.77
1:B:191:PRO:CB	1:B:361:PHE:CE1	2.60	0.77
1:A:199:THR:O	1:A:343:ILE:HD12	1.85	0.77
1:B:7:PHE:O	1:B:148:ALA:HA	1.85	0.77
1:B:287:PHE:O	1:B:288:ALA:CB	2.33	0.77
1:A:156:GLY:O	1:A:157:THR:CG2	2.29	0.76
1:A:139:VAL:CG1	1:A:145:LYS:HG2	2.15	0.76
1:B:247:THR:HG23	1:B:248:ASN:N	2.00	0.76
1:A:473:ILE:HG23	1:A:542:VAL:HG23	1.67	0.76
1:B:155:VAL:O	1:B:155:VAL:CG2	2.29	0.76
1:A:439:LEU:HD23	1:A:439:LEU:H	1.46	0.76
1:B:54:ILE:HD11	1:B:85:ASN:ND2	2.01	0.76
1:A:30:GLN:HA	1:A:30:GLN:NE2	2.01	0.76
1:B:45:MET:HG2	1:B:377:TYR:HE2	1.51	0.76
1:B:165:ILE:HG22	1:B:341:TYR:HA	1.68	0.76
1:A:288:ALA:C	1:A:291:ASN:CB	2.54	0.76
1:B:483:THR:HG22	1:B:529:PHE:HE1	1.51	0.75
1:B:247:THR:HG23	1:B:248:ASN:H	1.50	0.75
1:B:356:THR:O	1:B:357:LEU:HB2	1.87	0.75
1:A:122:GLN:CG	1:A:122:GLN:O	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLU:O	1:B:132:ASN:HB2	1.86	0.75
1:B:252:HIS:CD2	1:B:284:VAL:HG11	2.16	0.75
1:B:459:ASP:O	1:B:461:GLU:N	2.20	0.75
1:B:476:GLU:O	1:B:476:GLU:CG	2.35	0.75
1:A:347:PHE:O	1:A:347:PHE:CD1	2.39	0.75
1:A:424:GLU:CD	1:A:436:ARG:NH2	2.40	0.75
1:B:197:LEU:HD12	1:B:345:TYR:HB2	1.68	0.74
1:B:511:ASP:OD1	1:B:514:ARG:NH2	2.20	0.74
1:A:96:ARG:CG	1:A:96:ARG:HH11	2.01	0.74
1:B:90:PRO:CB	1:B:440:ARG:HD2	2.14	0.74
1:A:389:LEU:HD22	1:A:457:LEU:HD11	1.69	0.74
1:A:27:ARG:NH2	1:A:67:GLY:C	2.40	0.74
1:A:424:GLU:OE1	1:A:436:ARG:NH2	2.20	0.74
1:B:72:LYS:O	1:B:73:ALA:C	2.25	0.74
1:A:465:ARG:NH1	1:A:535:ASP:OD2	2.17	0.74
1:B:210:ILE:HD13	1:B:331:MET:HE1	1.69	0.74
1:B:461:GLU:CG	1:B:461:GLU:O	2.35	0.74
1:B:241:PRO:HB2	1:B:243:TYR:HE2	1.52	0.74
1:A:262:SER:HB2	1:A:263:PRO:CD	2.15	0.74
1:A:210:ILE:HG22	1:A:212:PHE:CD2	2.23	0.73
1:B:320:VAL:O	1:B:324:ILE:HG13	1.88	0.73
1:B:58:HIS:CE1	1:B:429:PHE:CZ	2.75	0.73
1:A:389:LEU:HD13	1:A:457:LEU:HD21	1.69	0.73
1:A:103:LEU:O	1:A:106:GLN:HB3	1.87	0.73
1:B:416:ASP:O	1:B:420:LEU:HD12	1.88	0.73
1:B:156:GLY:C	1:B:157:THR:CG2	2.57	0.73
1:A:200:GLY:HA2	1:A:342:ALA:HA	1.70	0.73
1:A:13:GLY:HA3	1:A:154:THR:CG2	2.18	0.73
1:A:204:ARG:HB2	1:A:338:ARG:HB2	1.71	0.72
1:B:20:GLU:HG3	1:B:381:ALA:HB1	1.71	0.72
1:A:404:ALA:CB	1:A:407:GLN:CG	2.55	0.72
1:A:129:ILE:HG22	1:A:136:VAL:HG13	1.71	0.72
1:B:389:LEU:HD11	1:B:455:LEU:HD13	1.72	0.72
1:A:289:ASP:C	1:A:291:ASN:O	2.28	0.72
1:B:27:ARG:HH11	1:B:27:ARG:HG2	1.55	0.72
1:A:385:LEU:HD23	1:A:385:LEU:C	2.09	0.72
1:B:190:LEU:HD11	1:B:362:ILE:HD11	1.70	0.72
1:A:28:MET:HE2	1:A:392:ALA:HB1	1.71	0.72
1:B:155:VAL:HG13	1:B:155:VAL:O	1.87	0.72
1:A:440:ARG:NH2	1:A:544:ILE:CG2	2.51	0.72
1:B:431:SER:O	1:B:432:ARG:C	2.27	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:THR:HG22	1:B:529:PHE:CE1	2.25	0.71
1:A:382:ALA:HB1	1:A:410:LEU:CD2	2.20	0.71
1:B:101:ARG:NH1	1:B:300:GLU:CD	2.42	0.71
1:B:24:ALA:HA	1:B:27:ARG:NH1	2.06	0.71
1:A:62:GLU:OE1	1:A:408:ALA:HB1	1.91	0.71
1:B:210:ILE:HG21	1:B:212:PHE:CE2	2.22	0.71
1:B:239:GLN:C	1:B:240:VAL:HG12	2.11	0.71
1:A:432:ARG:HB2	1:A:436:ARG:HH12	1.50	0.71
1:B:292:GLN:HA	1:B:292:GLN:HE21	1.56	0.71
1:A:413:LEU:HD11	1:A:417:LEU:HD11	1.72	0.71
1:B:401:TRP:CH2	1:B:403:PRO:HB3	2.25	0.71
1:A:2:PHE:CD1	1:A:145:LYS:HB2	2.25	0.71
1:B:389:LEU:HD13	1:B:457:LEU:HD11	1.71	0.71
1:B:405:ARG:HG2	1:B:405:ARG:O	1.90	0.71
1:B:155:VAL:HG11	1:B:371:ILE:HB	1.73	0.70
1:B:191:PRO:HG2	1:B:361:PHE:CE1	2.26	0.70
1:B:126:GLU:O	1:B:182:PRO:HG2	1.90	0.70
1:A:209:THR:HB	1:A:334:ALA:CA	2.19	0.70
1:B:127:ASP:HB2	1:B:182:PRO:HG2	1.74	0.70
1:B:45:MET:CG	1:B:377:TYR:CE2	2.72	0.70
1:B:252:HIS:CD2	1:B:284:VAL:CG1	2.71	0.70
1:B:159:LEU:HB3	1:B:160:ASP:HA	1.73	0.70
1:B:160:ASP:CG	1:B:161:GLY:N	2.44	0.70
1:A:203:PRO:HD2	1:A:203:PRO:O	1.90	0.70
1:B:100:ASP:OD2	1:B:103:LEU:HD12	1.92	0.70
1:A:39:ILE:HD12	1:A:122:GLN:HB2	1.73	0.70
1:A:10:ILE:HG12	1:A:33:LEU:HB3	1.74	0.69
1:A:-3:GLN:O	1:A:-2:GLY:C	2.30	0.69
1:B:9:VAL:HG21	1:B:25:ALA:HB1	1.72	0.69
1:A:511:ASP:HA	1:A:514:ARG:HH21	1.57	0.69
1:B:309:PRO:HB2	1:B:312:ILE:HD11	1.74	0.69
1:B:78:GLY:CA	1:B:98:GLN:O	2.41	0.69
1:A:28:MET:HE1	1:A:392:ALA:HB3	1.74	0.69
1:A:468:GLU:O	1:A:472:ASN:HB2	1.92	0.69
1:B:470:LEU:O	1:B:473:ILE:N	2.19	0.69
1:A:222:ASN:HD22	1:A:223:PRO:HA	1.58	0.69
1:A:284:VAL:C	1:A:286:ARG:N	2.41	0.69
1:B:45:MET:CE	1:B:104:TYR:CD1	2.77	0.69
1:B:2:PHE:O	1:B:3:TYR:O	2.10	0.68
1:B:347:PHE:CD1	1:B:373:GLY:HA3	2.29	0.68
1:A:393:ARG:HH21	1:A:399:GLU:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASN:HD22	1:A:383:GLN:NE2	1.91	0.68
1:A:453:ARG:HG2	1:A:463:TRP:CD2	2.29	0.68
1:A:13:GLY:HA3	1:A:154:THR:HG23	1.74	0.68
1:B:394:LEU:CD2	1:B:394:LEU:C	2.61	0.68
1:B:61:LYS:HG3	1:B:441:GLU:HG2	1.75	0.68
1:A:28:MET:CE	1:A:392:ALA:HB3	2.24	0.68
1:A:404:ALA:HB3	1:A:407:GLN:CD	2.13	0.68
1:B:467:ASN:O	1:B:470:LEU:N	2.22	0.68
1:A:473:ILE:HG23	1:A:542:VAL:CG2	2.24	0.68
1:A:45:MET:HE1	1:A:49:PRO:HA	1.74	0.68
1:A:102:VAL:HG12	1:A:103:LEU:N	2.09	0.68
1:B:-3:GLN:C	1:B:-1:SER:H	1.96	0.68
1:A:435:TYR:C	1:A:436:ARG:O	2.30	0.68
1:B:393:ARG:O	1:B:396:ASP:N	2.26	0.68
1:A:154:THR:O	1:A:155:VAL:CB	2.40	0.67
1:B:10:ILE:HB	1:B:151:VAL:HG22	1.77	0.67
1:B:55:GLY:O	1:B:58:HIS:HB2	1.94	0.67
1:A:365:LEU:HG	1:A:367:PHE:HE1	1.59	0.67
1:A:351:ARG:CD	1:A:421:GLY:HA3	2.24	0.67
1:A:13:GLY:C	1:A:154:THR:HG21	2.13	0.67
1:B:205:ILE:HG23	1:B:206:ASP:N	2.09	0.67
1:B:409:TYR:CE2	1:B:429:PHE:HE1	2.13	0.67
1:B:542:VAL:HG12	1:B:543:GLU:N	2.07	0.67
1:A:206:ASP:OD1	1:A:208:ARG:HD3	1.95	0.67
1:A:33:LEU:HD12	1:A:34:LEU:N	2.10	0.67
1:A:408:ALA:HA	1:A:447:ARG:HH21	1.60	0.66
1:B:190:LEU:HB3	1:B:191:PRO:HD2	1.76	0.66
1:A:48:ASN:HB2	1:A:49:PRO:HD2	1.76	0.66
1:B:451:ILE:O	1:B:455:LEU:HB2	1.96	0.66
1:A:115:GLN:HG3	1:A:115:GLN:O	1.95	0.66
1:B:230:MET:CE	1:B:230:MET:CA	2.71	0.66
1:A:293:HIS:O	1:A:294:GLN:C	2.34	0.66
1:B:109:ARG:O	1:B:111:ALA:N	2.28	0.66
1:A:458:VAL:HG13	1:A:462:ARG:HD2	1.78	0.66
1:B:310:ASN:HD22	1:B:311:GLY:N	1.94	0.66
1:A:234:SER:OG	1:A:235:GLN:N	2.29	0.66
1:A:28:MET:HE2	1:A:392:ALA:CB	2.26	0.66
1:B:295:ILE:HD11	1:B:311:GLY:O	1.96	0.66
1:B:347:PHE:CE1	1:B:373:GLY:HA3	2.31	0.66
1:A:165:ILE:C	1:A:166:GLY:O	2.31	0.66
1:B:80:GLN:OE1	1:B:242:CYS:SG	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PHE:CD1	1:B:373:GLY:CA	2.79	0.65
1:B:372:ASN:HD22	1:B:383:GLN:HE22	1.42	0.65
1:B:80:GLN:H	1:B:239:GLN:NE2	1.93	0.65
1:A:217:GLN:NE2	1:A:219:HIS:NE2	2.44	0.65
1:A:314:THR:HG21	1:A:316:LEU:CB	2.13	0.65
1:A:-3:GLN:O	1:A:-3:GLN:CG	2.30	0.65
1:A:95:THR:CG2	1:A:227:PHE:CE2	2.80	0.65
1:B:206:ASP:HB3	1:B:209:THR:HG23	1.78	0.65
1:B:314:THR:HG23	1:B:316:LEU:CB	2.26	0.65
1:B:409:TYR:CZ	1:B:429:PHE:HE1	2.14	0.65
1:A:347:PHE:C	1:A:347:PHE:CD1	2.67	0.65
1:B:292:GLN:CA	1:B:292:GLN:HE21	2.09	0.65
1:A:481:LYS:O	1:A:483:THR:N	2.29	0.65
1:B:70:MET:CG	1:B:70:MET:O	2.44	0.65
1:A:2:PHE:O	1:A:3:TYR:C	2.32	0.65
1:B:180:SER:C	1:B:181:ILE:HG22	2.14	0.65
1:B:81:PHE:CZ	1:B:236:HIS:CD2	2.85	0.65
1:B:356:THR:HG22	1:B:390:ASN:OD1	1.96	0.65
1:B:243:TYR:N	1:B:243:TYR:CD2	2.64	0.65
1:A:481:LYS:C	1:A:483:THR:H	2.00	0.65
1:A:52:GLY:HA2	1:A:56:LYS:HB3	1.78	0.65
1:A:155:VAL:HG12	1:A:156:GLY:H	1.61	0.64
1:A:285:MET:N	1:A:285:MET:HE2	1.99	0.64
1:B:226:VAL:CG2	1:B:232:ASN:HA	2.26	0.64
1:A:417:LEU:N	1:A:417:LEU:HD23	2.11	0.64
1:A:244:ILE:HD13	1:A:296:PHE:CE1	2.32	0.64
1:B:154:THR:CG2	1:B:155:VAL:N	2.31	0.64
1:B:38:ASN:HD22	1:B:40:ASP:H	1.45	0.64
1:A:203:PRO:CB	1:A:340:GLY:H	2.06	0.64
1:B:251:THR:O	1:B:255:ILE:HG13	1.97	0.64
1:B:241:PRO:HB2	1:B:243:TYR:CE2	2.32	0.64
1:B:241:PRO:CB	1:B:243:TYR:CE2	2.80	0.64
1:A:219:HIS:CE1	1:A:241:PRO:HB3	2.32	0.64
1:A:82:ARG:HA	1:A:221:ASP:OD1	1.97	0.64
1:A:203:PRO:CD	1:A:203:PRO:O	2.44	0.64
1:A:155:VAL:HG12	1:A:156:GLY:N	2.12	0.64
1:B:247:THR:CG2	1:B:248:ASN:N	2.60	0.64
1:A:405:ARG:HD2	1:A:415:ASP:OD2	1.97	0.64
1:A:282:ASP:OD1	1:A:286:ARG:NH1	2.30	0.64
1:B:-3:GLN:O	1:B:-1:SER:N	2.27	0.64
1:A:289:ASP:C	1:A:291:ASN:C	2.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:CA	1:A:154:THR:CG2	2.76	0.63
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.12	0.63
1:A:432:ARG:O	1:A:434:GLU:N	2.32	0.63
1:A:314:THR:CG2	1:A:316:LEU:N	2.53	0.63
1:B:314:THR:HG21	1:B:316:LEU:HB2	1.79	0.63
1:A:201:THR:CG2	1:A:202:PRO:HD2	2.29	0.63
1:B:191:PRO:CG	1:B:361:PHE:HE1	2.10	0.63
1:B:399:GLU:OE1	1:B:400:GLY:N	2.29	0.63
1:B:58:HIS:CE1	1:B:429:PHE:HZ	2.14	0.63
1:B:197:LEU:CD1	1:B:345:TYR:HB2	2.28	0.63
1:B:205:ILE:CG2	1:B:206:ASP:N	2.60	0.63
1:B:446:LEU:HD23	1:B:466:PHE:CZ	2.33	0.63
1:B:210:ILE:HD13	1:B:331:MET:CE	2.29	0.63
1:A:166:GLY:CA	1:A:315:SER:O	2.47	0.63
1:B:195:GLY:HA3	1:B:347:PHE:CE2	2.34	0.63
1:B:38:ASN:C	1:B:40:ASP:H	2.01	0.63
1:A:392:ALA:O	1:A:395:SER:N	2.31	0.63
1:A:430:THR:O	1:A:433:ALA:HB3	1.98	0.62
1:A:28:MET:CE	1:A:392:ALA:CB	2.77	0.62
1:A:48:ASN:HB2	1:A:49:PRO:CD	2.29	0.62
1:A:206:ASP:HB2	1:A:337:VAL:CG2	2.29	0.62
1:A:408:ALA:HB2	1:A:448:LEU:HD11	1.81	0.62
1:A:343:ILE:N	1:A:343:ILE:HD12	2.15	0.62
1:B:15:GLY:O	1:B:19:THR:OG1	2.13	0.62
1:A:343:ILE:HD12	1:A:343:ILE:H	1.64	0.62
1:B:453:ARG:NH1	1:B:463:TRP:HB2	2.14	0.62
1:B:379:GLU:O	1:B:383:GLN:HG3	2.00	0.62
1:B:222:ASN:HA	1:B:223:PRO:C	2.20	0.62
1:B:54:ILE:HD11	1:B:85:ASN:HD21	1.64	0.62
1:A:95:THR:HG22	1:A:227:PHE:HE2	1.63	0.62
1:B:126:GLU:HB3	1:B:139:VAL:O	2.00	0.62
1:A:209:THR:CB	1:A:334:ALA:HA	2.23	0.62
1:B:318:PHE:CE1	1:B:336:ILE:HG21	2.35	0.62
1:B:377:TYR:CD1	1:B:377:TYR:N	2.68	0.62
1:B:394:LEU:HD23	1:B:394:LEU:O	1.99	0.62
1:B:248:ASN:OD1	1:B:250:LYS:HB2	2.00	0.61
1:B:401:TRP:CE2	1:B:403:PRO:HB3	2.34	0.61
1:B:122:GLN:O	1:B:123:GLN:HG2	2.00	0.61
1:A:108:VAL:O	1:A:112:LEU:CD1	2.46	0.61
1:B:158:PHE:O	1:B:159:LEU:O	2.17	0.61
1:B:165:ILE:CG2	1:B:341:TYR:CB	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-3:GLN:C	1:B:-1:SER:N	2.53	0.61
1:A:11:ILE:HG13	1:A:22:ALA:HB2	1.82	0.61
1:B:194:VAL:CG2	1:B:348:PHE:CE1	2.83	0.61
1:B:522:LYS:O	1:B:525:THR:HB	2.00	0.61
1:B:38:ASN:C	1:B:40:ASP:N	2.52	0.61
1:B:366:PHE:CD1	1:B:391:ALA:HB2	2.35	0.61
1:B:287:PHE:O	1:B:288:ALA:HB2	1.99	0.61
1:A:201:THR:HG22	1:A:202:PRO:CD	2.29	0.61
1:B:544:ILE:O	1:B:548:TYR:HD1	1.84	0.61
1:B:7:PHE:N	1:B:147:ARG:O	2.28	0.61
1:A:191:PRO:HG2	1:A:361:PHE:CE2	2.35	0.61
1:A:37:HIS:NE2	1:A:157:THR:HG23	2.15	0.61
1:A:312:ILE:HG21	1:A:328:MET:CE	2.19	0.61
1:A:210:ILE:HG22	1:A:212:PHE:CE2	2.36	0.61
1:A:341:TYR:N	1:A:341:TYR:HD1	1.99	0.61
1:A:247:THR:HG22	1:A:293:HIS:N	2.10	0.61
1:B:62:GLU:HG2	1:B:448:LEU:HD12	1.82	0.61
1:B:127:ASP:O	1:B:138:ALA:HB1	2.01	0.60
1:A:202:PRO:HA	1:A:313:SER:HA	1.81	0.60
1:B:290:ARG:HD2	1:B:291:ASN:HD22	1.65	0.60
1:A:300:GLU:HB2	1:A:306:GLU:O	2.02	0.60
1:B:79:ILE:O	1:B:79:ILE:CG1	2.49	0.60
1:A:530:ALA:HB1	1:A:531:PRO:CA	2.30	0.60
1:B:201:THR:HG21	1:B:341:TYR:CE1	2.36	0.60
1:A:491:ALA:C	1:A:493:ALA:H	2.02	0.60
1:B:318:PHE:HE1	1:B:336:ILE:HG21	1.65	0.60
1:A:96:ARG:CG	1:A:96:ARG:NH1	2.63	0.60
1:B:163:ILE:HD12	1:B:163:ILE:H	1.66	0.60
1:B:282:ASP:C	1:B:284:VAL:H	2.04	0.60
1:A:465:ARG:HD2	1:A:465:ARG:O	2.01	0.60
1:A:53:GLY:N	1:A:96:ARG:HB3	2.17	0.60
1:A:351:ARG:CD	1:A:421:GLY:CA	2.71	0.60
1:A:75:ASP:OD1	1:A:236:HIS:HE1	1.85	0.60
1:A:215:LEU:HD13	1:A:245:THR:HG22	1.81	0.60
1:B:492:ALA:O	1:B:496:ASN:ND2	2.35	0.60
1:A:425:PRO:HB2	1:A:428:MET:CG	2.32	0.60
1:B:38:ASN:HA	1:B:122:GLN:OE1	2.01	0.60
1:B:247:THR:HB	1:B:293:HIS:O	2.00	0.60
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.66	0.60
1:A:153:LEU:HD22	1:A:154:THR:N	2.17	0.60
1:A:445:ASP:OD2	1:A:469:LYS:NZ	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:SER:O	1:B:512:LEU:HD23	2.02	0.59
1:A:393:ARG:HH11	1:A:455:LEU:CD2	2.15	0.59
1:A:203:PRO:HB3	1:A:321:GLN:OE1	2.02	0.59
1:A:72:LYS:O	1:A:75:ASP:HB2	2.03	0.59
1:A:139:VAL:HG13	1:A:145:LYS:CG	2.32	0.59
1:B:109:ARG:O	1:B:110:THR:C	2.41	0.59
1:A:425:PRO:HB2	1:A:428:MET:HG2	1.83	0.59
1:B:37:HIS:ND1	1:B:38:ASN:HB2	2.17	0.59
1:A:448:LEU:O	1:A:451:ILE:CG1	2.47	0.59
1:A:408:ALA:O	1:A:411:GLY:N	2.35	0.59
1:A:341:TYR:CD1	1:A:341:TYR:N	2.71	0.59
1:B:79:ILE:HA	1:B:239:GLN:HE21	1.65	0.59
1:A:240:VAL:HG23	1:A:241:PRO:N	2.18	0.59
1:B:154:THR:O	1:B:155:VAL:CB	2.50	0.59
1:B:72:LYS:O	1:B:75:ASP:N	2.36	0.59
1:A:247:THR:CG2	1:A:293:HIS:H	2.09	0.59
1:A:228:SER:OG	1:A:229:PHE:N	2.34	0.59
1:A:477:ARG:NH1	1:A:545:GLN:OE1	2.36	0.59
1:B:165:ILE:CG2	1:B:341:TYR:HB3	2.33	0.59
1:A:211:ASP:O	1:A:211:ASP:OD1	2.21	0.58
1:A:446:LEU:HD13	1:A:541:GLN:NE2	2.18	0.58
1:B:426:TYR:O	1:B:427:ARG:C	2.40	0.58
1:A:199:THR:HG22	1:A:343:ILE:HD13	1.85	0.58
1:A:152:VAL:HG22	1:A:366:PHE:HB2	1.84	0.58
1:A:349:ASP:OD1	1:A:350:PRO:HD2	2.03	0.58
1:A:527:THR:N	1:A:528:PRO:CD	2.67	0.58
1:B:360:LYS:C	1:B:361:PHE:HD2	2.05	0.58
1:A:230:MET:CE	1:A:230:MET:HA	2.33	0.58
1:B:191:PRO:HB2	1:B:361:PHE:CZ	2.37	0.58
1:A:61:LYS:HG3	1:A:441:GLU:HG2	1.85	0.58
1:A:106:GLN:O	1:A:110:THR:HG23	2.03	0.58
1:B:37:HIS:CE1	1:B:38:ASN:HB2	2.37	0.58
1:B:48:ASN:HB3	1:B:308:TYR:HE2	1.63	0.58
1:A:210:ILE:CG2	1:A:212:PHE:CE2	2.86	0.58
1:A:278:PRO:CG	1:A:279:SER:H	2.16	0.58
1:B:188:ARG:HH11	1:B:188:ARG:HB2	1.66	0.58
1:A:42:LEU:O	1:A:105:ARG:HG2	2.04	0.58
1:B:443:ASN:OD1	1:B:447:ARG:NH1	2.37	0.58
1:A:17:ALA:HB2	1:A:380:ALA:HB1	1.85	0.58
1:B:158:PHE:C	1:B:159:LEU:O	2.40	0.58
1:B:110:THR:O	1:B:114:ASN:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ALA:C	1:A:493:ALA:N	2.57	0.58
1:B:404:ALA:O	1:B:406:SER:N	2.28	0.58
1:B:30:GLN:N	1:B:30:GLN:HE21	2.01	0.57
1:B:537:GLN:O	1:B:540:GLU:HB3	2.04	0.57
1:B:48:ASN:ND2	1:B:50:ALA:HB3	2.18	0.57
1:B:452:GLY:O	1:B:453:ARG:C	2.43	0.57
1:A:465:ARG:HH12	1:A:535:ASP:CG	2.08	0.57
1:B:326:ARG:HH21	1:B:333:ASN:HA	1.69	0.57
1:B:232:ASN:N	1:B:232:ASN:HD22	2.02	0.57
1:B:95:THR:N	1:B:441:GLU:OE2	2.37	0.57
1:B:70:MET:HG2	1:B:70:MET:O	2.03	0.57
1:A:389:LEU:HD21	1:A:455:LEU:HD13	1.86	0.57
1:B:12:ILE:HG22	1:B:12:ILE:O	2.04	0.57
1:A:448:LEU:HD23	1:A:451:ILE:CD1	2.20	0.57
1:B:243:TYR:N	1:B:243:TYR:HD2	2.01	0.57
1:A:10:ILE:HG13	1:A:148:ALA:HB2	1.87	0.57
1:B:409:TYR:CZ	1:B:429:PHE:CE1	2.93	0.57
1:A:289:ASP:HA	1:A:291:ASN:C	2.25	0.57
1:A:45:MET:HE1	1:A:50:ALA:N	2.20	0.57
1:B:156:GLY:C	1:B:157:THR:HG22	2.25	0.57
1:A:453:ARG:HG2	1:A:463:TRP:CZ2	2.39	0.57
1:A:53:GLY:CA	1:A:96:ARG:HB3	2.35	0.57
1:A:404:ALA:HB3	1:A:407:GLN:CB	2.34	0.56
1:A:491:ALA:HB1	1:A:494:GLU:HB3	1.87	0.56
1:A:95:THR:HG22	1:A:227:PHE:CE2	2.39	0.56
1:B:183:LEU:O	1:B:187:LEU:HD22	2.04	0.56
1:B:194:VAL:HG22	1:B:348:PHE:CD1	2.41	0.56
1:B:314:THR:CG2	1:B:316:LEU:N	2.68	0.56
1:B:80:GLN:H	1:B:239:GLN:HE22	1.52	0.56
1:A:319:ASP:N	1:A:319:ASP:OD2	2.38	0.56
1:B:81:PHE:O	1:B:82:ARG:O	2.23	0.56
1:A:513:LEU:HD23	1:A:546:VAL:HG11	1.88	0.56
1:A:45:MET:HE1	1:A:49:PRO:C	2.25	0.56
1:B:415:ASP:O	1:B:417:LEU:N	2.39	0.56
1:A:33:LEU:HD12	1:A:119:MET:O	2.05	0.56
1:A:45:MET:CE	1:A:49:PRO:CA	2.75	0.56
1:B:228:SER:OG	1:B:230:MET:N	2.37	0.56
1:B:81:PHE:HB3	1:B:225:PRO:CG	2.33	0.56
1:B:165:ILE:HG23	1:B:341:TYR:CB	2.36	0.56
1:A:240:VAL:HG21	1:A:299:PRO:HG2	1.87	0.56
1:B:484:TRP:CE3	1:B:508:SER:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:HD2	1:B:338:ARG:HD3	1.88	0.56
1:B:73:ALA:CB	1:B:104:TYR:CE2	2.89	0.56
1:A:127:ASP:HA	1:A:183:LEU:HB2	1.88	0.56
1:A:261:ARG:O	1:A:262:SER:O	2.23	0.56
1:B:191:PRO:HD2	1:B:361:PHE:CD1	2.41	0.55
1:B:306:GLU:OE1	1:B:338:ARG:NH1	2.39	0.55
1:B:279:SER:HB2	1:B:282:ASP:HB2	1.88	0.55
1:B:427:ARG:NH2	1:B:428:MET:CE	2.68	0.55
1:B:127:ASP:OD2	1:B:186:ARG:NH1	2.40	0.55
1:B:356:THR:O	1:B:357:LEU:CB	2.52	0.55
1:A:45:MET:HE1	1:A:49:PRO:CA	2.36	0.55
1:B:190:LEU:CB	1:B:191:PRO:CD	2.84	0.55
1:B:64:ASP:OD2	1:B:462:ARG:NH2	2.37	0.55
1:B:69:LEU:O	1:B:71:ALA:N	2.40	0.55
1:B:380:ALA:O	1:B:381:ALA:C	2.42	0.55
1:B:205:ILE:HD11	1:B:336:ILE:HG13	1.89	0.55
1:B:486:THR:C	1:B:488:SER:H	2.10	0.55
1:A:496:ASN:HD22	1:A:502:PRO:HB3	1.72	0.55
1:A:85:ASN:O	1:A:93:ARG:HD3	2.05	0.55
1:A:155:VAL:HG11	1:A:370:GLN:HE21	1.72	0.55
1:B:98:GLN:HE22	1:B:298:GLU:HG2	1.72	0.55
1:B:349:ASP:OD2	1:B:351:ARG:NH1	2.39	0.55
1:B:306:GLU:CD	1:B:338:ARG:NH1	2.61	0.55
1:B:48:ASN:CB	1:B:308:TYR:CE2	2.83	0.55
1:A:123:GLN:HG3	1:A:142:MET:HE1	1.88	0.55
1:A:207:ALA:HB2	1:A:305:ASN:O	2.07	0.55
1:B:181:ILE:O	1:B:181:ILE:HG23	2.07	0.55
1:A:310:ASN:C	1:A:310:ASN:HD22	2.10	0.55
1:A:316:LEU:HD13	1:A:320:VAL:HG11	1.89	0.55
1:B:424:GLU:OE2	1:B:436:ARG:NH2	2.36	0.55
1:B:440:ARG:NH2	1:B:442:ASP:OD1	2.35	0.55
1:B:194:VAL:HG22	1:B:348:PHE:CE1	2.42	0.54
1:B:371:ILE:HG23	1:B:372:ASN:N	2.22	0.54
1:B:234:SER:O	1:B:236:HIS:N	2.40	0.54
1:B:320:VAL:HG12	1:B:324:ILE:HD11	1.89	0.54
1:A:38:ASN:ND2	1:A:40:ASP:H	2.04	0.54
1:B:140:THR:HG21	1:B:146:PHE:HE2	1.71	0.54
1:A:209:THR:HG21	1:A:335:LYS:HG3	0.83	0.54
1:B:476:GLU:HG2	1:B:533:LEU:HD22	1.88	0.54
1:A:70:MET:CE	1:A:381:ALA:HB2	2.37	0.54
1:B:524:THR:HG21	1:B:532:ALA:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD21	1:A:512:LEU:HD21	1.88	0.54
1:B:337:VAL:HG12	1:B:338:ARG:HG3	1.90	0.54
1:A:440:ARG:NH1	1:A:440:ARG:HG3	2.23	0.54
1:A:240:VAL:HG23	1:A:241:PRO:O	2.08	0.54
1:B:525:THR:HG22	1:B:526:LEU:HD23	1.88	0.54
1:B:162:LYS:O	1:B:343:ILE:HG22	2.06	0.54
1:A:211:ASP:C	1:A:213:SER:H	2.10	0.54
1:B:33:LEU:HD12	1:B:119:MET:HG2	1.89	0.54
1:A:278:PRO:CD	1:A:279:SER:H	2.21	0.54
1:B:252:HIS:CD2	1:B:284:VAL:HG13	2.43	0.54
1:A:72:LYS:O	1:A:73:ALA:C	2.46	0.54
1:B:35:LEU:CD1	1:B:125:VAL:HG23	2.38	0.54
1:B:241:PRO:HB3	1:B:243:TYR:CE2	2.43	0.54
1:A:469:LYS:HE3	1:A:537:GLN:HG2	1.90	0.54
1:A:436:ARG:O	1:A:437:LEU:CB	2.51	0.54
1:A:155:VAL:CG1	1:A:370:GLN:HE21	2.19	0.54
1:A:79:ILE:HD11	1:A:299:PRO:HB2	1.90	0.54
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.73	0.54
1:A:488:SER:O	1:A:492:ALA:HB2	2.08	0.54
1:B:139:VAL:CG1	1:B:145:LYS:HG2	2.19	0.54
1:A:408:ALA:HA	1:A:447:ARG:NH2	2.21	0.54
1:B:317:PRO:HD2	1:B:320:VAL:HG21	1.90	0.54
1:A:351:ARG:HD2	1:A:420:LEU:C	2.27	0.54
1:B:404:ALA:O	1:B:407:GLN:N	2.28	0.54
1:A:485:VAL:HG23	1:A:503:LEU:CD1	2.38	0.54
1:B:372:ASN:HD22	1:B:383:GLN:NE2	2.06	0.54
1:B:190:LEU:CB	1:B:191:PRO:HD2	2.38	0.54
1:A:437:LEU:HD12	1:A:437:LEU:C	2.29	0.53
1:A:293:HIS:CD2	1:A:293:HIS:N	2.75	0.53
1:A:127:ASP:OD1	1:A:186:ARG:NH1	2.42	0.53
1:A:536:GLU:OE1	1:A:536:GLU:HA	2.07	0.53
1:A:203:PRO:O	1:A:205:ILE:HD13	2.09	0.53
1:B:190:LEU:HB3	1:B:191:PRO:CD	2.39	0.53
1:A:2:PHE:CE1	1:A:145:LYS:HB3	2.43	0.53
1:B:96:ARG:CG	1:B:96:ARG:O	2.47	0.53
1:B:292:GLN:HA	1:B:292:GLN:NE2	2.22	0.53
1:A:70:MET:HE3	1:A:381:ALA:HB2	1.90	0.53
1:B:366:PHE:CD1	1:B:366:PHE:N	2.75	0.53
1:B:410:LEU:O	1:B:414:VAL:HG23	2.08	0.53
1:A:33:LEU:C	1:A:33:LEU:HD12	2.28	0.53
1:A:484:TRP:N	1:A:484:TRP:CD1	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD11	1:A:331:MET:HE1	1.89	0.53
1:B:385:LEU:C	1:B:385:LEU:HD23	2.29	0.53
1:A:187:LEU:O	1:A:190:LEU:HG	2.09	0.53
1:B:399:GLU:OE1	1:B:399:GLU:HA	2.09	0.53
1:A:413:LEU:CD1	1:A:417:LEU:HD11	2.39	0.53
1:B:62:GLU:CD	1:B:408:ALA:HB1	2.28	0.53
1:B:404:ALA:O	1:B:407:GLN:HB2	2.08	0.53
1:A:440:ARG:HH11	1:A:440:ARG:HG3	1.74	0.53
1:A:474:GLU:O	1:A:475:ARG:C	2.46	0.53
1:B:362:ILE:O	1:B:363:GLN:C	2.47	0.53
1:A:377:TYR:O	1:A:380:ALA:N	2.40	0.53
1:A:485:VAL:HG23	1:A:503:LEU:HD13	1.89	0.53
1:B:440:ARG:O	1:B:443:ASN:OD1	2.27	0.53
1:B:81:PHE:CD2	1:B:236:HIS:HD2	2.27	0.53
1:B:446:LEU:HD23	1:B:466:PHE:CE1	2.44	0.53
1:A:404:ALA:CB	1:A:407:GLN:CD	2.77	0.52
1:A:205:ILE:CG2	1:A:210:ILE:CD1	2.85	0.52
1:A:314:THR:CG2	1:A:315:SER:H	2.08	0.52
1:A:30:GLN:CA	1:A:30:GLN:NE2	2.70	0.52
1:B:62:GLU:HG2	1:B:448:LEU:CD1	2.38	0.52
1:A:196:ARG:NH2	1:A:344:GLU:HB3	2.25	0.52
1:A:354:LYS:C	1:A:356:THR:H	2.11	0.52
1:A:284:VAL:O	1:A:285:MET:C	2.42	0.52
1:B:318:PHE:HA	1:B:321:GLN:HG3	1.91	0.52
1:B:37:HIS:ND1	1:B:37:HIS:O	2.41	0.52
1:A:453:ARG:NH1	1:A:463:TRP:HB2	2.25	0.52
1:A:109:ARG:NH1	1:B:303:THR:O	2.41	0.52
1:B:238:GLN:HB3	1:B:302:LEU:HD11	1.92	0.52
1:A:445:ASP:OD1	1:A:445:ASP:N	2.42	0.52
1:A:469:LYS:O	1:A:473:ILE:HD12	2.09	0.52
1:A:11:ILE:HG13	1:A:22:ALA:CA	2.39	0.52
1:A:289:ASP:O	1:A:291:ASN:O	2.27	0.52
1:B:409:TYR:HA	1:B:412:VAL:HG23	1.92	0.52
1:A:512:LEU:HD12	1:A:529:PHE:CE2	2.44	0.52
1:B:129:ILE:O	1:B:136:VAL:HG12	2.10	0.52
1:A:49:PRO:HD2	1:A:298:GLU:OE1	2.09	0.52
1:B:255:ILE:HG23	1:B:316:LEU:HD11	1.90	0.52
1:B:470:LEU:O	1:B:471:GLU:C	2.47	0.52
1:B:226:VAL:HG12	1:B:227:PHE:N	2.24	0.52
1:A:393:ARG:NH1	1:A:455:LEU:CD2	2.73	0.52
1:B:2:PHE:CE2	1:B:145:LYS:HE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:CA	1:A:154:THR:HG21	2.39	0.52
1:B:385:LEU:HD21	1:B:457:LEU:CD1	2.40	0.52
1:A:385:LEU:HD23	1:A:385:LEU:O	2.10	0.52
1:B:35:LEU:HD12	1:B:125:VAL:HG23	1.92	0.51
1:B:385:LEU:HD21	1:B:457:LEU:HD13	1.91	0.51
1:A:8:ASP:HB3	1:A:395:SER:HB2	1.92	0.51
1:A:155:VAL:CG1	1:A:156:GLY:H	2.14	0.51
1:B:426:TYR:O	1:B:429:PHE:N	2.40	0.51
1:B:415:ASP:O	1:B:416:ASP:C	2.49	0.51
1:A:95:THR:HG21	1:A:227:PHE:CE2	2.46	0.51
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.43	0.51
1:B:295:ILE:CD1	1:B:311:GLY:O	2.58	0.51
1:B:205:ILE:HG23	1:B:206:ASP:H	1.75	0.51
1:A:248:ASN:O	1:A:251:THR:N	2.44	0.51
1:A:486:THR:O	1:A:488:SER:N	2.44	0.51
1:B:539:ALA:O	1:B:540:GLU:C	2.49	0.51
1:B:104:TYR:O	1:B:107:ALA:N	2.34	0.51
1:B:51:ILE:HD12	1:B:74:ILE:HG12	1.93	0.51
1:A:153:LEU:CD2	1:A:154:THR:N	2.74	0.51
1:A:153:LEU:CD2	1:A:154:THR:H	2.23	0.51
1:A:316:LEU:HD13	1:A:320:VAL:CG1	2.41	0.51
1:B:358:GLU:N	1:B:366:PHE:CD2	2.79	0.51
1:B:518:MET:HE2	1:B:519:THR:H	1.76	0.51
1:A:129:ILE:HB	1:A:137:GLY:O	2.11	0.51
1:B:30:GLN:HA	1:B:30:GLN:NE2	2.26	0.51
1:B:30:GLN:CA	1:B:30:GLN:NE2	2.74	0.51
1:B:130:VAL:HG21	1:B:186:ARG:HE	1.76	0.51
1:B:379:GLU:N	1:B:379:GLU:OE1	2.28	0.51
1:A:262:SER:CB	1:A:263:PRO:HD3	2.34	0.51
1:A:206:ASP:N	1:A:337:VAL:HG23	2.25	0.51
1:A:2:PHE:CE1	1:A:145:LYS:CB	2.94	0.51
1:B:259:LEU:C	1:B:261:ARG:H	2.14	0.51
1:A:154:THR:HG23	1:A:155:VAL:N	2.26	0.50
1:A:262:SER:OG	1:A:263:PRO:N	2.39	0.50
1:B:159:LEU:HB3	1:B:160:ASP:CA	2.41	0.50
1:A:460:ASP:O	1:A:461:GLU:C	2.48	0.50
1:B:56:LYS:O	1:B:60:VAL:HG23	2.11	0.50
1:A:161:GLY:O	1:A:162:LYS:O	2.29	0.50
1:B:437:LEU:HG	1:B:437:LEU:O	2.12	0.50
1:A:251:THR:O	1:A:255:ILE:HD12	2.11	0.50
1:B:422:THR:HG22	1:B:422:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:CD	1:A:447:ARG:HH22	2.15	0.50
1:B:228:SER:OG	1:B:229:PHE:N	2.45	0.50
1:B:284:VAL:HG12	1:B:284:VAL:O	2.11	0.50
1:A:471:GLU:O	1:A:472:ASN:C	2.46	0.50
1:A:185:ARG:O	1:A:186:ARG:C	2.49	0.50
1:A:429:PHE:CD2	1:A:429:PHE:C	2.84	0.50
1:B:393:ARG:O	1:B:394:LEU:C	2.50	0.50
1:B:19:THR:HG23	1:B:112:LEU:HD11	1.92	0.50
1:A:287:PHE:HD1	1:A:288:ALA:H	1.59	0.50
1:B:232:ASN:N	1:B:232:ASN:ND2	2.58	0.50
1:B:12:ILE:C	1:B:154:THR:CG2	2.75	0.50
1:A:155:VAL:O	1:A:156:GLY:O	2.30	0.50
1:A:62:GLU:CD	1:A:408:ALA:HB1	2.31	0.50
1:B:156:GLY:O	1:B:157:THR:O	2.30	0.50
1:A:199:THR:HG22	1:A:343:ILE:CD1	2.42	0.50
1:A:203:PRO:HB3	1:A:340:GLY:N	2.15	0.50
1:A:474:GLU:O	1:A:476:GLU:N	2.44	0.50
1:B:165:ILE:CG2	1:B:341:TYR:HA	2.41	0.50
1:A:234:SER:C	1:A:236:HIS:H	2.16	0.50
1:A:60:VAL:HG11	1:A:227:PHE:CE1	2.46	0.50
1:B:239:GLN:C	1:B:240:VAL:CG1	2.80	0.50
1:B:349:ASP:OD1	1:B:349:ASP:C	2.50	0.50
1:A:90:PRO:HA	1:A:93:ARG:HG3	1.94	0.49
1:B:459:ASP:O	1:B:462:ARG:N	2.41	0.49
1:A:488:SER:O	1:A:489:ALA:O	2.30	0.49
1:B:83:ILE:HG22	1:B:83:ILE:O	2.11	0.49
1:A:101:ARG:HD2	1:A:300:GLU:OE2	2.12	0.49
1:A:255:ILE:HG21	1:A:281:GLU:HA	1.95	0.49
1:B:159:LEU:HA	1:B:160:ASP:O	2.12	0.49
1:A:408:ALA:O	1:A:409:TYR:C	2.49	0.49
1:B:322:MET:O	1:B:326:ARG:HB2	2.13	0.49
1:B:106:GLN:O	1:B:106:GLN:HG3	2.12	0.49
1:A:289:ASP:CA	1:A:291:ASN:C	2.81	0.49
1:B:194:VAL:CG2	1:B:348:PHE:HE1	2.24	0.49
1:B:366:PHE:C	1:B:367:PHE:HD1	2.16	0.49
1:B:331:MET:N	1:B:332:GLU:OE1	2.45	0.49
1:B:300:GLU:OE2	1:B:308:TYR:HD1	1.96	0.49
1:B:417:LEU:O	1:B:421:GLY:CA	2.53	0.49
1:A:479:ARG:HA	1:A:482:SER:HB2	1.95	0.49
1:A:423:LYS:HE3	1:A:424:GLU:O	2.12	0.49
1:A:165:ILE:O	1:A:166:GLY:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLN:CA	1:B:292:GLN:NE2	2.75	0.49
1:B:366:PHE:CE1	1:B:391:ALA:CB	2.90	0.49
1:B:165:ILE:HG22	1:B:341:TYR:CA	2.41	0.49
1:A:378:GLU:N	1:A:378:GLU:OE1	2.43	0.49
1:B:19:THR:O	1:B:23:MET:HB2	2.13	0.49
1:A:316:LEU:HD22	1:A:320:VAL:HG11	1.95	0.49
1:B:318:PHE:CE1	1:B:336:ILE:HD13	2.48	0.49
1:B:408:ALA:CB	1:B:448:LEU:HD11	2.43	0.49
1:A:43:GLY:HA3	1:A:105:ARG:HA	1.95	0.49
1:B:440:ARG:O	1:B:447:ARG:NH1	2.46	0.49
1:B:431:SER:C	1:B:433:ALA:N	2.65	0.49
1:B:200:GLY:HA2	1:B:342:ALA:HA	1.95	0.49
1:B:154:THR:C	1:B:155:VAL:CG1	2.52	0.48
1:A:379:GLU:OE2	1:A:426:TYR:OH	2.26	0.48
1:A:314:THR:CG2	1:A:316:LEU:CB	2.84	0.48
1:A:-3:GLN:O	1:A:-2:GLY:O	2.30	0.48
1:B:458:VAL:HG13	1:B:462:ARG:HD2	1.94	0.48
1:B:71:ALA:O	1:B:72:LYS:C	2.50	0.48
1:A:167:LEU:O	1:A:168:ASP:OD1	2.31	0.48
1:A:310:ASN:C	1:A:310:ASN:ND2	2.65	0.48
1:B:205:ILE:HD12	1:B:336:ILE:HA	1.87	0.48
1:A:469:LYS:HG2	1:A:473:ILE:HD11	1.95	0.48
1:A:458:VAL:HG12	1:A:459:ASP:N	2.29	0.48
1:A:430:THR:O	1:A:433:ALA:CB	2.61	0.48
1:A:53:GLY:N	1:A:96:ARG:CB	2.77	0.48
1:A:385:LEU:C	1:A:385:LEU:CD2	2.81	0.48
1:A:9:VAL:O	1:A:32:THR:HA	2.12	0.48
1:B:65:ALA:HB1	1:B:449:THR:OG1	2.13	0.48
1:A:289:ASP:HA	1:A:291:ASN:O	2.13	0.48
1:B:194:VAL:CG2	1:B:348:PHE:CD1	2.97	0.48
1:A:432:ARG:O	1:A:433:ALA:C	2.51	0.48
1:B:520:TYR:HB3	1:B:543:GLU:OE2	2.13	0.48
1:A:365:LEU:HG	1:A:367:PHE:CE1	2.46	0.48
1:B:188:ARG:NH1	1:B:188:ARG:HB2	2.28	0.48
1:A:463:TRP:O	1:A:466:PHE:HB3	2.13	0.48
1:B:363:GLN:HE21	1:B:363:GLN:HB3	1.45	0.48
1:A:453:ARG:HA	1:A:453:ARG:HD2	1.65	0.48
1:B:371:ILE:HG23	1:B:372:ASN:H	1.79	0.48
1:A:204:ARG:HD3	1:A:338:ARG:HD2	1.96	0.48
1:B:81:PHE:O	1:B:225:PRO:CG	2.62	0.48
1:B:81:PHE:CZ	1:B:236:HIS:NE2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLU:OE2	1:A:363:GLN:HB3	2.13	0.48
1:A:519:THR:O	1:A:520:TYR:C	2.52	0.48
1:B:473:ILE:HG23	1:B:542:VAL:HG23	1.95	0.47
1:B:24:ALA:HA	1:B:27:ARG:HH11	1.75	0.47
1:B:408:ALA:HB2	1:B:448:LEU:HD11	1.96	0.47
1:B:386:LEU:HD12	1:B:389:LEU:CD2	2.35	0.47
1:B:508:SER:O	1:B:512:LEU:CD2	2.62	0.47
1:A:393:ARG:HH21	1:A:398:LYS:HB3	1.79	0.47
1:A:295:ILE:CD1	1:A:311:GLY:HA3	2.44	0.47
1:A:314:THR:CG2	1:A:315:SER:N	2.48	0.47
1:A:448:LEU:CG	1:A:451:ILE:HD11	2.44	0.47
1:B:128:LEU:HA	1:B:138:ALA:HB2	1.96	0.47
1:A:441:GLU:O	1:A:443:ASN:N	2.46	0.47
1:A:247:THR:O	1:A:248:ASN:HB3	2.14	0.47
1:A:64:ASP:O	1:A:67:GLY:N	2.39	0.47
1:A:230:MET:HE3	1:A:230:MET:HA	1.96	0.47
1:A:413:LEU:C	1:A:413:LEU:HD12	2.34	0.47
1:A:444:ALA:O	1:A:448:LEU:HB2	2.14	0.47
1:B:183:LEU:HG	1:B:183:LEU:O	2.14	0.47
1:A:153:LEU:HD22	1:A:154:THR:H	1.78	0.47
1:B:331:MET:HB2	1:B:334:ALA:HB2	1.96	0.47
1:B:393:ARG:NE	1:B:399:GLU:O	2.44	0.47
1:B:431:SER:HB2	1:B:432:ARG:H	1.43	0.47
1:B:239:GLN:O	1:B:240:VAL:HG12	2.14	0.47
1:A:392:ALA:O	1:A:395:SER:OG	2.25	0.47
1:B:165:ILE:HG23	1:B:341:TYR:HB2	1.96	0.47
1:A:11:ILE:HD12	1:A:21:ALA:CB	2.44	0.47
1:A:89:GLY:CA	1:A:93:ARG:HE	2.28	0.47
1:B:450:GLU:C	1:B:452:GLY:N	2.65	0.47
1:B:201:THR:HG21	1:B:341:TYR:CD1	2.49	0.47
1:B:222:ASN:ND2	1:B:223:PRO:HA	2.21	0.47
1:B:299:PRO:HA	1:B:307:ILE:HD12	1.96	0.47
1:B:410:LEU:O	1:B:413:LEU:HB3	2.15	0.47
1:A:16:HIS:O	1:A:17:ALA:C	2.53	0.47
1:B:322:MET:O	1:B:323:GLN:C	2.54	0.47
1:A:154:THR:O	1:A:155:VAL:HB	2.12	0.46
1:A:541:GLN:HE21	1:A:545:GLN:HE21	1.62	0.46
1:B:357:LEU:O	1:B:358:GLU:C	2.53	0.46
1:B:385:LEU:O	1:B:385:LEU:HD23	2.15	0.46
1:B:65:ALA:HA	1:B:462:ARG:NH1	2.29	0.46
1:A:526:LEU:C	1:A:528:PRO:HD2	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:VAL:O	1:A:413:LEU:C	2.54	0.46
1:B:51:ILE:HB	1:B:74:ILE:HG13	1.97	0.46
1:B:48:ASN:HA	1:B:49:PRO:HD3	1.66	0.46
1:B:542:VAL:CG1	1:B:543:GLU:N	2.75	0.46
1:B:518:MET:SD	1:B:523:LEU:HD12	2.55	0.46
1:A:24:ALA:O	1:A:25:ALA:C	2.53	0.46
1:B:197:LEU:HD12	1:B:345:TYR:CB	2.41	0.46
1:A:11:ILE:HG13	1:A:22:ALA:CB	2.45	0.46
1:B:56:LYS:HD3	1:B:378:GLU:CD	2.36	0.46
1:B:91:ALA:H	1:B:440:ARG:HD2	1.80	0.46
1:B:409:TYR:CE1	1:B:439:LEU:HB3	2.50	0.46
1:A:116:PRO:O	1:A:117:ASN:HB2	2.15	0.46
1:B:467:ASN:O	1:B:468:GLU:C	2.53	0.46
1:A:423:LYS:HE2	1:A:426:TYR:CE2	2.51	0.46
1:A:410:LEU:O	1:A:410:LEU:HD13	2.15	0.46
1:B:64:ASP:OD1	1:B:228:SER:HB2	2.15	0.46
1:A:81:PHE:HB3	1:A:225:PRO:CG	2.29	0.46
1:A:463:TRP:CE3	1:A:463:TRP:HA	2.50	0.46
1:A:219:HIS:ND1	1:A:241:PRO:HB3	2.30	0.46
1:A:377:TYR:O	1:A:378:GLU:C	2.53	0.46
1:B:13:GLY:CA	1:B:154:THR:CG2	2.77	0.46
1:A:423:LYS:HG2	1:A:424:GLU:O	2.16	0.46
1:A:295:ILE:CD1	1:A:312:ILE:HG23	2.45	0.46
1:B:459:ASP:C	1:B:461:GLU:N	2.68	0.46
1:A:294:GLN:HB2	1:A:294:GLN:HE21	1.58	0.46
1:A:123:GLN:HG3	1:A:142:MET:CE	2.45	0.46
1:B:348:PHE:N	1:B:371:ILE:O	2.49	0.46
1:B:379:GLU:O	1:B:380:ALA:C	2.54	0.46
1:B:357:LEU:HA	1:B:357:LEU:HD23	1.77	0.46
1:B:459:ASP:O	1:B:460:ASP:C	2.54	0.46
1:A:460:ASP:O	1:A:462:ARG:N	2.49	0.46
1:B:215:LEU:HD21	1:B:329:GLN:HG2	1.98	0.46
1:B:2:PHE:HE2	1:B:145:LYS:HE3	1.82	0.46
1:B:444:ALA:HA	1:B:447:ARG:NH1	2.31	0.46
1:B:240:VAL:HA	1:B:241:PRO:HD2	1.62	0.46
1:B:287:PHE:O	1:B:288:ALA:HB3	2.13	0.46
1:A:393:ARG:NH2	1:A:398:LYS:HB3	2.30	0.46
1:B:301:GLY:O	1:B:303:THR:N	2.49	0.46
1:B:290:ARG:HD2	1:B:291:ASN:ND2	2.28	0.46
1:A:338:ARG:NH2	1:B:39:ILE:HB	2.12	0.45
1:A:481:LYS:N	1:A:481:LYS:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ALA:O	1:A:490:GLU:C	2.54	0.45
1:B:158:PHE:CD1	1:B:158:PHE:O	2.68	0.45
1:A:186:ARG:HH11	1:A:186:ARG:CB	2.30	0.45
1:A:289:ASP:CA	1:A:291:ASN:O	2.65	0.45
1:B:295:ILE:HA	1:B:295:ILE:HD13	1.62	0.45
1:A:70:MET:HE3	1:A:381:ALA:CB	2.46	0.45
1:A:259:LEU:O	1:A:261:ARG:N	2.50	0.45
1:A:278:PRO:HG2	1:A:279:SER:H	1.79	0.45
1:B:215:LEU:CD2	1:B:329:GLN:HG2	2.46	0.45
1:B:77:ALA:O	1:B:99:ALA:HA	2.17	0.45
1:A:208:ARG:O	1:A:210:ILE:N	2.50	0.45
1:B:505:ARG:O	1:B:507:ALA:N	2.50	0.45
1:B:367:PHE:CD1	1:B:367:PHE:N	2.84	0.45
1:B:445:ASP:O	1:B:449:THR:HB	2.16	0.45
1:B:427:ARG:NH2	1:B:428:MET:HE2	2.31	0.45
1:B:416:ASP:OD1	1:B:420:LEU:HD11	2.17	0.45
1:A:484:TRP:HA	1:A:508:SER:HA	1.98	0.45
1:A:287:PHE:HB3	1:A:288:ALA:O	2.16	0.45
1:A:92:VAL:HG21	1:A:430:THR:HG23	1.99	0.45
1:A:440:ARG:NH2	1:A:544:ILE:HG22	2.30	0.45
1:B:386:LEU:O	1:B:389:LEU:HB3	2.17	0.45
1:B:64:ASP:OD2	1:B:462:ARG:NH1	2.46	0.45
1:B:31:GLN:HA	1:B:31:GLN:HE21	1.77	0.45
1:A:7:PHE:CD2	1:A:33:LEU:HB2	2.52	0.45
1:B:9:VAL:HA	1:B:150:ALA:O	2.16	0.45
1:B:116:PRO:O	1:B:117:ASN:HB2	2.17	0.45
1:A:354:LYS:C	1:A:356:THR:N	2.69	0.45
1:A:9:VAL:HG22	1:A:150:ALA:HB3	1.99	0.45
1:B:44:GLN:HB2	1:B:44:GLN:HE21	1.55	0.45
1:A:37:HIS:CD2	1:A:157:THR:HG23	2.52	0.45
1:A:312:ILE:HG13	1:A:312:ILE:O	2.17	0.45
1:B:321:GLN:HA	1:B:324:ILE:HD12	1.99	0.45
1:B:430:THR:CG2	1:B:431:SER:N	2.80	0.45
1:A:53:GLY:HA2	1:A:96:ARG:HB3	1.99	0.45
1:B:371:ILE:CG2	1:B:372:ASN:H	2.29	0.44
1:A:54:ILE:CD1	1:A:85:ASN:HD21	2.30	0.44
1:A:91:ALA:HB2	1:A:437:LEU:HD13	1.99	0.44
1:B:38:ASN:O	1:B:39:ILE:C	2.52	0.44
1:A:372:ASN:ND2	1:A:383:GLN:HE21	2.08	0.44
1:A:166:GLY:CA	1:A:317:PRO:HG3	2.33	0.44
1:A:474:GLU:HB3	1:A:475:ARG:H	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASP:HB3	1:B:209:THR:CG2	2.46	0.44
1:B:390:ASN:HA	1:B:390:ASN:HD22	1.41	0.44
1:B:28:MET:HG3	1:B:457:LEU:HD23	1.98	0.44
1:B:81:PHE:CD2	1:B:236:HIS:CD2	3.03	0.44
1:A:467:ASN:HA	1:A:470:LEU:HB3	1.99	0.44
1:B:124:ALA:HB3	1:B:141:GLN:HB3	1.99	0.44
1:A:310:ASN:HD22	1:A:311:GLY:N	2.15	0.44
1:A:474:GLU:O	1:A:477:ARG:N	2.49	0.44
1:B:205:ILE:HD11	1:B:336:ILE:CG1	2.47	0.44
1:B:247:THR:O	1:B:248:ASN:HB3	2.18	0.44
1:B:450:GLU:O	1:B:451:ILE:C	2.54	0.44
1:B:303:THR:O	1:B:303:THR:OG1	2.36	0.44
1:A:52:GLY:N	1:A:378:GLU:OE2	2.43	0.44
1:B:222:ASN:C	1:B:223:PRO:O	2.55	0.44
1:A:11:ILE:HG21	1:A:18:GLY:O	2.17	0.44
1:A:59:LEU:HA	1:A:59:LEU:HD12	1.87	0.44
1:B:245:THR:HG23	1:B:246:HIS:N	2.33	0.44
1:B:495:VAL:HG11	1:B:503:LEU:HD11	1.99	0.44
1:A:202:PRO:CA	1:A:313:SER:HA	2.46	0.44
1:B:90:PRO:HG3	1:B:544:ILE:HG23	1.98	0.44
1:B:205:ILE:HD13	1:B:205:ILE:HA	1.47	0.44
1:B:484:TRP:HA	1:B:508:SER:HA	1.98	0.44
1:A:380:ALA:O	1:A:381:ALA:C	2.56	0.44
1:A:215:LEU:N	1:A:215:LEU:HD23	2.32	0.44
1:A:80:GLN:HE21	1:A:98:GLN:HG2	1.82	0.44
1:A:396:ASP:OD1	1:A:396:ASP:O	2.35	0.44
1:B:280:ILE:C	1:B:282:ASP:H	2.19	0.44
1:A:84:LEU:N	1:A:94:ALA:O	2.51	0.44
1:B:500:THR:HG23	1:B:501:ALA:N	2.32	0.44
1:B:81:PHE:HB3	1:B:225:PRO:HD2	2.00	0.44
1:A:232:ASN:N	1:A:235:GLN:OE1	2.44	0.44
1:B:28:MET:CE	1:B:392:ALA:HB3	2.47	0.44
1:B:405:ARG:HG3	1:B:412:VAL:HA	2.00	0.44
1:A:207:ALA:CB	1:A:305:ASN:O	2.66	0.44
1:B:137:GLY:HA3	1:B:146:PHE:O	2.18	0.44
1:B:495:VAL:O	1:B:499:LEU:HD23	2.18	0.44
1:A:41:THR:OG1	1:A:157:THR:OG1	2.34	0.44
1:A:27:ARG:HH22	1:A:68:GLY:N	2.15	0.44
1:B:496:ASN:HB3	1:B:502:PRO:HB3	2.00	0.44
1:A:202:PRO:HG3	1:A:308:TYR:CE2	2.53	0.44
1:B:191:PRO:CD	1:B:361:PHE:CE1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:OG1	1:B:334:ALA:CA	2.44	0.44
1:B:396:ASP:O	1:B:396:ASP:OD1	2.36	0.44
1:A:473:ILE:HG13	1:A:538:ALA:HB1	2.00	0.44
1:A:542:VAL:HG12	1:A:543:GLU:N	2.33	0.44
1:A:27:ARG:NH2	1:A:68:GLY:N	2.65	0.44
1:A:481:LYS:C	1:A:483:THR:N	2.67	0.44
1:B:290:ARG:CD	1:B:291:ASN:HD22	2.31	0.44
1:B:141:GLN:O	1:B:141:GLN:HG2	2.17	0.44
1:B:130:VAL:HG21	1:B:186:ARG:NE	2.32	0.43
1:A:211:ASP:O	1:A:212:PHE:C	2.54	0.43
1:A:248:ASN:O	1:A:251:THR:OG1	2.17	0.43
1:A:38:ASN:O	1:A:40:ASP:N	2.51	0.43
1:A:246:HIS:CD2	1:A:246:HIS:N	2.84	0.43
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.83	0.43
1:B:234:SER:O	1:B:235:GLN:C	2.55	0.43
1:B:399:GLU:OE1	1:B:399:GLU:CA	2.66	0.43
1:B:300:GLU:OE2	1:B:308:TYR:CD1	2.71	0.43
1:A:2:PHE:CD1	1:A:145:LYS:CB	2.98	0.43
1:B:59:LEU:HA	1:B:59:LEU:HD12	1.64	0.43
1:A:153:LEU:HA	1:A:153:LEU:HD23	1.58	0.43
1:A:317:PRO:HD2	1:A:320:VAL:HG21	2.00	0.43
1:B:366:PHE:H	1:B:366:PHE:HD1	1.66	0.43
1:B:7:PHE:CE1	1:B:33:LEU:HD13	2.53	0.43
1:B:80:GLN:N	1:B:239:GLN:NE2	2.64	0.43
1:A:403:PRO:HG2	1:A:410:LEU:HD12	2.00	0.43
1:B:369:GLY:C	1:B:371:ILE:H	2.19	0.43
1:B:7:PHE:O	1:B:148:ALA:CA	2.61	0.43
1:B:195:GLY:O	1:B:346:ASP:HA	2.19	0.43
1:A:479:ARG:HG2	1:A:479:ARG:O	2.19	0.43
1:B:371:ILE:CG2	1:B:372:ASN:N	2.82	0.43
1:A:425:PRO:HD2	1:A:428:MET:CE	2.49	0.43
1:A:212:PHE:HD1	1:A:243:TYR:CG	2.36	0.43
1:A:408:ALA:CA	1:A:447:ARG:HH21	2.31	0.43
1:B:331:MET:HE2	1:B:331:MET:HB3	1.83	0.43
1:B:367:PHE:HD1	1:B:367:PHE:N	2.17	0.43
1:A:413:LEU:CD1	1:A:417:LEU:HD21	2.49	0.43
1:B:115:GLN:HG3	1:B:115:GLN:O	2.19	0.43
1:B:139:VAL:HG13	1:B:145:LYS:CD	2.47	0.43
1:A:166:GLY:HA2	1:A:315:SER:O	2.16	0.43
1:B:204:ARG:O	1:B:205:ILE:HD13	2.18	0.43
1:B:526:LEU:C	1:B:528:PRO:HD2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:O	1:A:91:ALA:N	2.51	0.43
1:A:243:TYR:HB2	1:A:297:LEU:HB2	2.00	0.43
1:A:81:PHE:CZ	1:A:236:HIS:CE1	3.07	0.43
1:A:80:GLN:O	1:A:97:ALA:HA	2.19	0.43
1:A:212:PHE:HD1	1:A:243:TYR:CD2	2.37	0.43
1:B:118:LEU:HD12	1:B:119:MET:N	2.34	0.43
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.87	0.43
1:A:56:LYS:HB3	1:A:378:GLU:HG2	2.01	0.43
1:A:38:ASN:C	1:A:38:ASN:ND2	2.70	0.43
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.52	0.43
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.63	0.43
1:B:10:ILE:HG12	1:B:33:LEU:HD23	2.01	0.43
1:B:238:GLN:HB3	1:B:302:LEU:CD1	2.49	0.43
1:A:230:MET:HA	1:A:230:MET:HE2	2.00	0.43
1:A:413:LEU:HD13	1:A:417:LEU:HD21	2.01	0.43
1:B:423:LYS:HG2	1:B:424:GLU:N	2.34	0.43
1:A:544:ILE:O	1:A:545:GLN:C	2.55	0.42
1:B:79:ILE:CA	1:B:239:GLN:NE2	2.71	0.42
1:B:302:LEU:HA	1:B:302:LEU:HD23	1.50	0.42
1:A:34:LEU:HD12	1:A:34:LEU:C	2.39	0.42
1:A:519:THR:O	1:A:522:LYS:N	2.52	0.42
1:A:41:THR:O	1:A:42:LEU:C	2.58	0.42
1:A:31:GLN:OE1	1:A:117:ASN:ND2	2.52	0.42
1:B:448:LEU:HA	1:B:448:LEU:HD23	1.77	0.42
1:B:423:LYS:HB3	1:B:423:LYS:HE3	1.80	0.42
1:B:386:LEU:HB3	1:B:387:ALA:H	1.70	0.42
1:B:98:GLN:HE22	1:B:298:GLU:CG	2.30	0.42
1:A:7:PHE:CD1	1:A:7:PHE:N	2.87	0.42
1:A:490:GLU:OE2	1:A:490:GLU:HA	2.19	0.42
1:A:354:LYS:O	1:A:356:THR:N	2.52	0.42
1:A:429:PHE:O	1:A:429:PHE:CD2	2.72	0.42
1:B:38:ASN:ND2	1:B:40:ASP:H	2.15	0.42
1:B:219:HIS:CE1	1:B:241:PRO:HD3	2.54	0.42
1:B:241:PRO:CB	1:B:243:TYR:HE2	2.17	0.42
1:B:100:ASP:OD2	1:B:302:LEU:HB2	2.19	0.42
1:B:485:VAL:HG11	1:B:528:PRO:HG3	2.02	0.42
1:B:299:PRO:HG2	1:B:299:PRO:O	2.18	0.42
1:B:126:GLU:HA	1:B:126:GLU:OE1	2.20	0.42
1:B:181:ILE:HA	1:B:182:PRO:HD2	1.79	0.42
1:B:539:ALA:O	1:B:541:GLN:N	2.52	0.42
1:B:-1:SER:OG	1:B:-1:SER:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG21	1:A:227:PHE:CD2	2.54	0.42
1:B:23:MET:CE	1:B:115:GLN:OE1	2.67	0.42
1:B:493:ALA:HA	1:B:496:ASN:HD22	1.84	0.42
1:B:365:LEU:CD2	1:B:367:PHE:HE1	2.32	0.42
1:B:413:LEU:O	1:B:414:VAL:C	2.58	0.42
1:B:242:CYS:HB3	1:B:297:LEU:O	2.19	0.42
1:B:439:LEU:HA	1:B:439:LEU:HD23	1.45	0.42
1:A:33:LEU:CD1	1:A:119:MET:O	2.68	0.42
1:A:278:PRO:CD	1:A:279:SER:N	2.82	0.42
1:B:305:ASN:N	1:B:305:ASN:OD1	2.48	0.42
1:B:190:LEU:N	1:B:190:LEU:HD23	2.35	0.42
1:B:314:THR:HG23	1:B:316:LEU:CA	2.49	0.42
1:A:463:TRP:HE3	1:A:463:TRP:HA	1.85	0.42
1:B:131:GLU:N	1:B:134:ARG:O	2.53	0.42
1:A:428:MET:SD	1:A:432:ARG:NH2	2.93	0.42
1:A:31:GLN:OE1	1:A:31:GLN:HA	2.19	0.42
1:B:316:LEU:HD22	1:B:320:VAL:HG11	2.02	0.42
1:A:393:ARG:HH11	1:A:455:LEU:HD23	1.83	0.42
1:A:27:ARG:NH2	1:A:67:GLY:CA	2.83	0.42
1:B:446:LEU:HD23	1:B:446:LEU:HA	1.89	0.42
1:B:251:THR:O	1:B:254:VAL:HB	2.20	0.41
1:B:314:THR:CG2	1:B:316:LEU:CB	2.84	0.41
1:B:79:ILE:O	1:B:79:ILE:HG13	2.20	0.41
1:B:80:GLN:H	1:B:239:GLN:CD	2.24	0.41
1:A:259:LEU:C	1:A:261:ARG:H	2.24	0.41
1:A:317:PRO:O	1:A:321:GLN:HG3	2.19	0.41
1:B:428:MET:O	1:B:429:PHE:C	2.57	0.41
1:B:508:SER:O	1:B:511:ASP:HB2	2.20	0.41
1:A:57:GLY:O	1:A:60:VAL:N	2.51	0.41
1:A:12:ILE:HG23	1:A:12:ILE:HD13	1.84	0.41
1:A:25:ALA:O	1:A:30:GLN:HB2	2.21	0.41
1:A:7:PHE:CE2	1:A:33:LEU:HB2	2.55	0.41
1:B:115:GLN:O	1:B:116:PRO:C	2.56	0.41
1:A:127:ASP:OD1	1:A:128:LEU:N	2.53	0.41
1:A:525:THR:HG23	1:A:525:THR:O	2.19	0.41
1:A:376:GLY:HA3	1:A:379:GLU:OE1	2.20	0.41
1:A:443:ASN:OD1	1:A:447:ARG:CD	2.54	0.41
1:B:450:GLU:HB3	1:B:463:TRP:CH2	2.56	0.41
1:B:425:PRO:HB2	1:B:428:MET:HG2	2.01	0.41
1:A:106:GLN:O	1:A:109:ARG:N	2.54	0.41
1:B:524:THR:CG2	1:B:532:ALA:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:PRO:HB3	1:B:503:LEU:O	2.20	0.41
1:A:295:ILE:HA	1:A:295:ILE:HD13	1.92	0.41
1:A:443:ASN:O	1:A:446:LEU:HB2	2.21	0.41
1:B:210:ILE:HG21	1:B:210:ILE:HD13	1.76	0.41
1:A:252:HIS:HD2	1:A:284:VAL:CG2	2.33	0.41
1:B:434:GLU:O	1:B:437:LEU:HB2	2.20	0.41
1:A:307:ILE:HA	1:A:307:ILE:HD12	1.72	0.41
1:A:280:ILE:O	1:A:284:VAL:HG23	2.21	0.41
1:A:422:THR:HG23	1:A:423:LYS:O	2.20	0.41
1:A:167:LEU:HG	1:A:167:LEU:H	1.39	0.41
1:B:449:THR:O	1:B:449:THR:CG2	2.69	0.41
1:A:81:PHE:HB2	1:A:225:PRO:HG2	1.98	0.41
1:A:230:MET:HB3	1:A:230:MET:HE2	1.71	0.41
1:A:129:ILE:N	1:A:137:GLY:O	2.42	0.41
1:B:24:ALA:HA	1:B:27:ARG:HG2	2.02	0.41
1:A:512:LEU:HD12	1:A:529:PHE:HE2	1.85	0.41
1:B:515:ARG:HA	1:B:516:PRO:HD3	1.93	0.41
1:B:362:ILE:O	1:B:363:GLN:O	2.38	0.41
1:A:224:MET:HA	1:A:225:PRO:HD2	1.62	0.41
1:B:396:ASP:CG	1:B:398:LYS:HE3	2.41	0.41
1:B:426:TYR:O	1:B:427:ARG:O	2.38	0.41
1:B:470:LEU:HD12	1:B:470:LEU:HA	1.65	0.41
1:B:127:ASP:HB2	1:B:182:PRO:CG	2.46	0.41
1:B:325:VAL:O	1:B:331:MET:HG3	2.20	0.41
1:B:390:ASN:HD21	1:B:401:TRP:H	1.67	0.41
1:A:104:TYR:CE1	1:A:108:VAL:HG21	2.56	0.41
1:A:247:THR:OG1	1:A:251:THR:HG21	2.21	0.41
1:B:446:LEU:HA	1:B:466:PHE:HZ	1.86	0.41
1:B:436:ARG:O	1:B:438:MET:N	2.48	0.41
1:A:289:ASP:H	1:A:291:ASN:HA	1.80	0.41
1:B:184:SER:O	1:B:185:ARG:C	2.59	0.41
1:A:370:GLN:C	1:A:372:ASN:N	2.70	0.41
1:A:203:PRO:HA	1:A:340:GLY:N	2.35	0.41
1:B:386:LEU:HD22	1:B:410:LEU:HD11	2.03	0.41
1:B:81:PHE:CB	1:B:225:PRO:HD2	2.51	0.41
1:B:284:VAL:CG1	1:B:284:VAL:O	2.69	0.41
1:A:392:ALA:O	1:A:395:SER:CB	2.69	0.41
1:A:466:PHE:C	1:A:466:PHE:CD1	2.94	0.41
1:A:11:ILE:HD12	1:A:21:ALA:HB3	2.03	0.41
1:A:120:ILE:HG22	1:A:121:PHE:N	2.36	0.41
1:A:426:TYR:O	1:A:427:ARG:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PRO:HG2	1:A:548:TYR:CD1	2.56	0.40
1:B:38:ASN:C	1:B:38:ASN:HD22	2.25	0.40
1:A:312:ILE:HD13	1:A:328:MET:HE1	2.03	0.40
1:A:206:ASP:OD1	1:A:208:ARG:N	2.49	0.40
1:A:159:LEU:CB	1:A:160:ASP:CA	2.92	0.40
1:B:417:LEU:HD23	1:B:422:THR:H	1.86	0.40
1:A:166:GLY:O	1:A:168:ASP:N	2.54	0.40
1:B:392:ALA:O	1:B:395:SER:OG	2.38	0.40
1:A:115:GLN:HA	1:A:116:PRO:HD2	1.08	0.40
1:A:202:PRO:HB2	1:A:203:PRO:CD	2.51	0.40
1:A:212:PHE:HD2	1:A:212:PHE:H	1.67	0.40
1:B:210:ILE:CD1	1:B:331:MET:CE	2.99	0.40
1:A:419:THR:HB	1:A:420:LEU:HG	2.02	0.40
1:B:222:ASN:CA	1:B:223:PRO:O	2.69	0.40
1:A:230:MET:HE1	1:A:465:ARG:HG2	2.04	0.40
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.91	0.40
1:A:232:ASN:O	1:A:235:GLN:HB2	2.22	0.40
1:B:98:GLN:HE22	1:B:298:GLU:CD	2.24	0.40
1:B:246:HIS:O	1:B:328:MET:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/576 (90%)	383 (74%)	88 (17%)	50 (10%)	1	10
1	B	518/576 (90%)	363 (70%)	98 (19%)	57 (11%)	0	8
All	All	1039/1152 (90%)	746 (72%)	186 (18%)	107 (10%)	1	9

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLY
1	A	142	MET
1	A	160	ASP
1	A	167	LEU
1	A	212	PHE
1	A	235	GLN
1	A	237	PRO
1	A	260	ASP
1	A	262	SER
1	A	285	MET
1	A	289	ASP
1	A	433	ALA
1	A	437	LEU
1	A	474	GLU
1	A	475	ARG
1	A	482	SER
1	A	490	GLU
1	B	39	ILE
1	B	80	GLN
1	B	82	ARG
1	B	90	PRO
1	B	91	ALA
1	B	155	VAL
1	B	158	PHE
1	B	159	LEU
1	B	160	ASP
1	B	235	GLN
1	B	241	PRO
1	B	283	LYS
1	B	287	PHE
1	B	288	ALA
1	B	357	LEU
1	B	363	GLN
1	B	405	ARG
1	B	432	ARG
1	B	460	ASP
1	B	490	GLU
1	B	502	PRO
1	B	506	GLU
1	B	535	ASP
1	B	540	GLU
1	A	-2	GLY
1	A	136	VAL

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Mol	Chain	Res	Type
1	A	156	GLY
1	A	159	LEU
1	A	162	LYS
1	A	166	GLY
1	A	397	ASP
1	A	487	PRO
1	A	489	ALA
1	A	494	GLU
1	A	502	PRO
1	B	-2	GLY
1	B	68	GLY
1	B	70	MET
1	B	110	THR
1	B	157	THR
1	B	279	SER
1	B	302	LEU
1	B	305	ASN
1	B	389	LEU
1	B	415	ASP
1	B	416	ASP
1	B	422	THR
1	B	427	ARG
1	B	431	SER
1	B	447	ARG
1	A	24	ALA
1	A	103	LEU
1	A	116	PRO
1	A	294	GLN
1	B	132	ASN
1	B	260	ASP
1	B	358	GLU
1	B	376	GLY
1	B	394	LEU
1	B	406	SER
1	B	539	ALA
1	A	209	THR
1	A	464	ALA
1	A	535	ASP
1	A	536	GLU
1	B	181	ILE
1	B	289	ASP
1	B	312	ILE

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Mol	Chain	Res	Type
1	A	17	ALA
1	A	141	GLN
1	A	181	ILE
1	A	436	ARG
1	A	442	ASP
1	A	517	GLU
1	B	144	LEU
1	B	254	VAL
1	B	499	LEU
1	B	536	GLU
1	A	4	PRO
1	A	39	ILE
1	A	106	GLN
1	A	107	ALA
1	A	155	VAL
1	A	161	GLY
1	A	412	VAL
1	B	3	TYR
1	B	386	LEU
1	B	487	PRO
1	A	54	ILE
1	B	452	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/474 (90%)	338 (79%)	88 (21%)	1	8
1	B	427/474 (90%)	320 (75%)	107 (25%)	1	4
All	All	853/948 (90%)	658 (77%)	195 (23%)	1	6

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	GLN

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Mol	Chain	Res	Type
1	A	-1	SER
1	A	2	PHE
1	A	5	ASP
1	A	12	ILE
1	A	31	GLN
1	A	39	ILE
1	A	44	GLN
1	A	49	PRO
1	A	54	ILE
1	A	69	LEU
1	A	70	MET
1	A	76	GLN
1	A	82	ARG
1	A	92	VAL
1	A	93	ARG
1	A	96	ARG
1	A	100	ASP
1	A	106	GLN
1	A	110	THR
1	A	115	GLN
1	A	125	VAL
1	A	136	VAL
1	A	139	VAL
1	A	153	LEU
1	A	155	VAL
1	A	167	LEU
1	A	181	ILE
1	A	184	SER
1	A	187	LEU
1	A	190	LEU
1	A	197	LEU
1	A	199	THR
1	A	209	THR
1	A	217	GLN
1	A	221	ASP
1	A	222	ASN
1	A	227	PHE
1	A	230	MET
1	A	244	ILE
1	A	245	THR
1	A	251	THR
1	A	257	SER

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Mol	Chain	Res	Type
1	A	262	SER
1	A	279	SER
1	A	280	ILE
1	A	282	ASP
1	A	285	MET
1	A	287	PHE
1	A	294	GLN
1	A	302	LEU
1	A	307	ILE
1	A	310	ASN
1	A	313	SER
1	A	319	ASP
1	A	322	MET
1	A	341	TYR
1	A	343	ILE
1	A	347	PHE
1	A	354	LYS
1	A	363	GLN
1	A	371	ILE
1	A	394	LEU
1	A	397	ASP
1	A	413	LEU
1	A	422	THR
1	A	428	MET
1	A	431	SER
1	A	432	ARG
1	A	434	GLU
1	A	437	LEU
1	A	438	MET
1	A	439	LEU
1	A	440	ARG
1	A	445	ASP
1	A	448	LEU
1	A	450	GLU
1	A	453	ARG
1	A	461	GLU
1	A	481	LYS
1	A	484	TRP
1	A	485	VAL
1	A	488	SER
1	A	502	PRO
1	A	527	THR

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Mol	Chain	Res	Type
1	A	534	THR
1	A	540	GLU
1	A	549	GLU
1	B	-3	GLN
1	B	2	PHE
1	B	9	VAL
1	B	27	ARG
1	B	30	GLN
1	B	33	LEU
1	B	35	LEU
1	B	37	HIS
1	B	38	ASN
1	B	39	ILE
1	B	44	GLN
1	B	46	SER
1	B	54	ILE
1	B	59	LEU
1	B	69	LEU
1	B	72	LYS
1	B	74	ILE
1	B	79	ILE
1	B	82	ARG
1	B	106	GLN
1	B	110	THR
1	B	114	ASN
1	B	119	MET
1	B	120	ILE
1	B	122	GLN
1	B	133	ASP
1	B	139	VAL
1	B	141	GLN
1	B	149	LYS
1	B	153	LEU
1	B	157	THR
1	B	163	ILE
1	B	180	SER
1	B	184	SER
1	B	186	ARG
1	B	187	LEU
1	B	190	LEU
1	B	193	ARG
1	B	197	LEU

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Mol	Chain	Res	Type
1	B	199	THR
1	B	205	ILE
1	B	208	ARG
1	B	209	THR
1	B	214	VAL
1	B	222	ASN
1	B	227	PHE
1	B	228	SER
1	B	230	MET
1	B	232	ASN
1	B	234	SER
1	B	238	GLN
1	B	240	VAL
1	B	243	TYR
1	B	245	THR
1	B	247	THR
1	B	251	THR
1	B	259	LEU
1	B	282	ASP
1	B	286	ARG
1	B	289	ASP
1	B	290	ARG
1	B	292	GLN
1	B	295	ILE
1	B	303	THR
1	B	304	SER
1	B	306	GLU
1	B	307	ILE
1	B	310	ASN
1	B	312	ILE
1	B	313	SER
1	B	314	THR
1	B	319	ASP
1	B	323	GLN
1	B	326	ARG
1	B	336	ILE
1	B	338	ARG
1	B	339	PRO
1	B	343	ILE
1	B	351	ARG
1	B	355	PRO
1	B	356	THR

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Mol	Chain	Res	Type
1	B	361	PHE
1	B	363	GLN
1	B	377	TYR
1	B	389	LEU
1	B	399	GLU
1	B	420	LEU
1	B	422	THR
1	B	430	THR
1	B	431	SER
1	B	432	ARG
1	B	470	LEU
1	B	471	GLU
1	B	474	GLU
1	B	476	GLU
1	B	481	LYS
1	B	484	TRP
1	B	499	LEU
1	B	502	PRO
1	B	512	LEU
1	B	513	LEU
1	B	518	MET
1	B	519	THR
1	B	534	THR
1	B	542	VAL
1	B	547	LYS
1	B	548	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	31	GLN
1	A	38	ASN
1	A	80	GLN
1	A	117	ASN
1	A	217	GLN
1	A	218	GLN
1	A	222	ASN
1	A	232	ASN
1	A	252	HIS
1	A	294	GLN
1	A	310	ASN

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Mol	Chain	Res	Type
1	A	363	GLN
1	A	370	GLN
1	A	383	GLN
1	A	390	ASN
1	A	541	GLN
1	B	30	GLN
1	B	31	GLN
1	B	38	ASN
1	B	44	GLN
1	B	85	ASN
1	B	98	GLN
1	B	117	ASN
1	B	217	GLN
1	B	222	ASN
1	B	232	ASN
1	B	236	HIS
1	B	239	GLN
1	B	252	HIS
1	B	291	ASN
1	B	292	GLN
1	B	310	ASN
1	B	363	GLN
1	B	383	GLN
1	B	390	ASN
1	B	545	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	551	-	4,4,4	0.29	0	6,6,6	0.32	0
2	SO4	A	552	-	4,4,4	0.24	0	6,6,6	0.42	0
2	SO4	B	1	-	4,4,4	0.18	0	6,6,6	0.50	0
2	SO4	B	551	-	4,4,4	0.13	0	6,6,6	0.26	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
2	SO4	A	551	-	-	0/0/0/0	0/0/0/0
2	SO4	A	552	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	551	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	551	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	527/576 (91%)	0.36	28 (5%)	30 23	53, 73, 123, 136	0
1	B	524/576 (90%)	0.57	52 (9%)	9 9	55, 79, 130, 137	0
All	All	1051/1152 (91%)	0.47	80 (7%)	17 14	53, 75, 128, 137	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	LEU	6.0
1	B	507	ALA	6.0
1	B	289	ASP	5.7
1	A	485	VAL	5.6
1	B	164	HIS	5.2
1	B	506	GLU	4.9
1	A	486	THR	4.9
1	A	507	ALA	4.6
1	B	485	VAL	4.4
1	A	498	HIS	4.3
1	A	491	ALA	4.0
1	B	499	LEU	4.0
1	B	503	LEU	4.0
1	A	518	MET	4.0
1	B	292	GLN	4.0
1	B	486	THR	3.9
1	B	498	HIS	3.9
1	A	180	SER	3.8
1	B	475	ARG	3.7
1	B	525	THR	3.7
1	A	504	SER	3.6
1	B	285	MET	3.6
1	B	286	ARG	3.6
1	A	506	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	532	ALA	3.4
1	B	484	TRP	3.4
1	A	499	LEU	3.3
1	B	479	ARG	3.2
1	B	472	ASN	3.2
1	B	523	LEU	3.2
1	B	500	THR	3.2
1	A	512	LEU	3.2
1	B	214	VAL	3.1
1	A	483	THR	3.1
1	B	480	LEU	3.1
1	A	527	THR	3.0
1	B	529	PHE	3.0
1	A	501	ALA	3.0
1	A	215	LEU	3.0
1	A	493	ALA	2.9
1	A	529	PHE	2.9
1	B	483	THR	2.9
1	A	484	TRP	2.9
1	B	284	VAL	2.8
1	B	288	ALA	2.8
1	B	512	LEU	2.8
1	B	491	ALA	2.8
1	A	482	SER	2.8
1	B	495	VAL	2.8
1	B	180	SER	2.7
1	B	527	THR	2.7
1	B	505	ARG	2.7
1	A	526	LEU	2.6
1	A	495	VAL	2.6
1	B	493	ALA	2.6
1	A	550	GLY	2.6
1	A	505	ARG	2.5
1	B	256	ARG	2.5
1	B	250	LYS	2.5
1	B	526	LEU	2.4
1	A	244	ILE	2.4
1	B	215	LEU	2.4
1	B	290	ARG	2.4
1	B	316	LEU	2.3
1	B	291	ASN	2.3
1	B	533	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	287	PHE	2.2
1	B	278	PRO	2.2
1	B	538	ALA	2.2
1	B	528	PRO	2.2
1	B	518	MET	2.1
1	B	261	ARG	2.1
1	A	289	ASP	2.1
1	B	243	TYR	2.1
1	B	510	GLU	2.0
1	B	191	PRO	2.0
1	A	497	ALA	2.0
1	B	329	GLN	2.0
1	B	474	GLU	2.0
1	B	509	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	1	5/5	0.96	0.25	-0.13	77,78,78,78	0
2	SO4	A	551	5/5	0.98	0.17	-0.88	71,72,72,72	0
2	SO4	A	552	5/5	0.93	0.20	-	79,79,79,80	0
2	SO4	B	551	5/5	0.93	0.20	-	85,85,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.