



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:29 PM UTC

PDB ID : 3G05 / pdb_00003g05
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

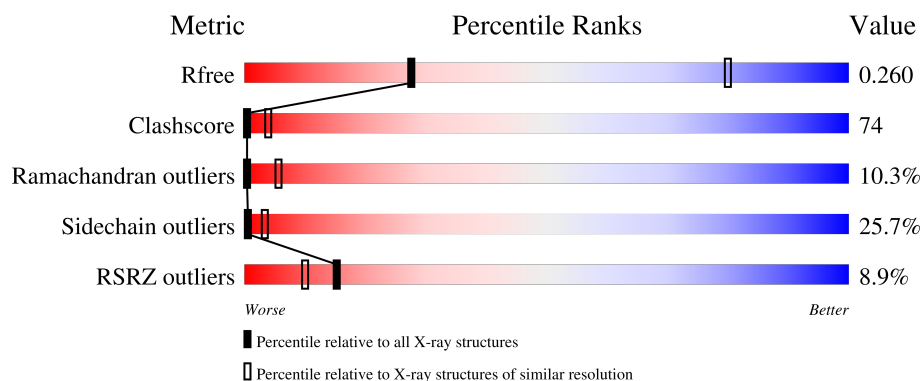
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	8% 20% 47% 19% 6% 9%
1	B	576	8% 18% 45% 23% 5% 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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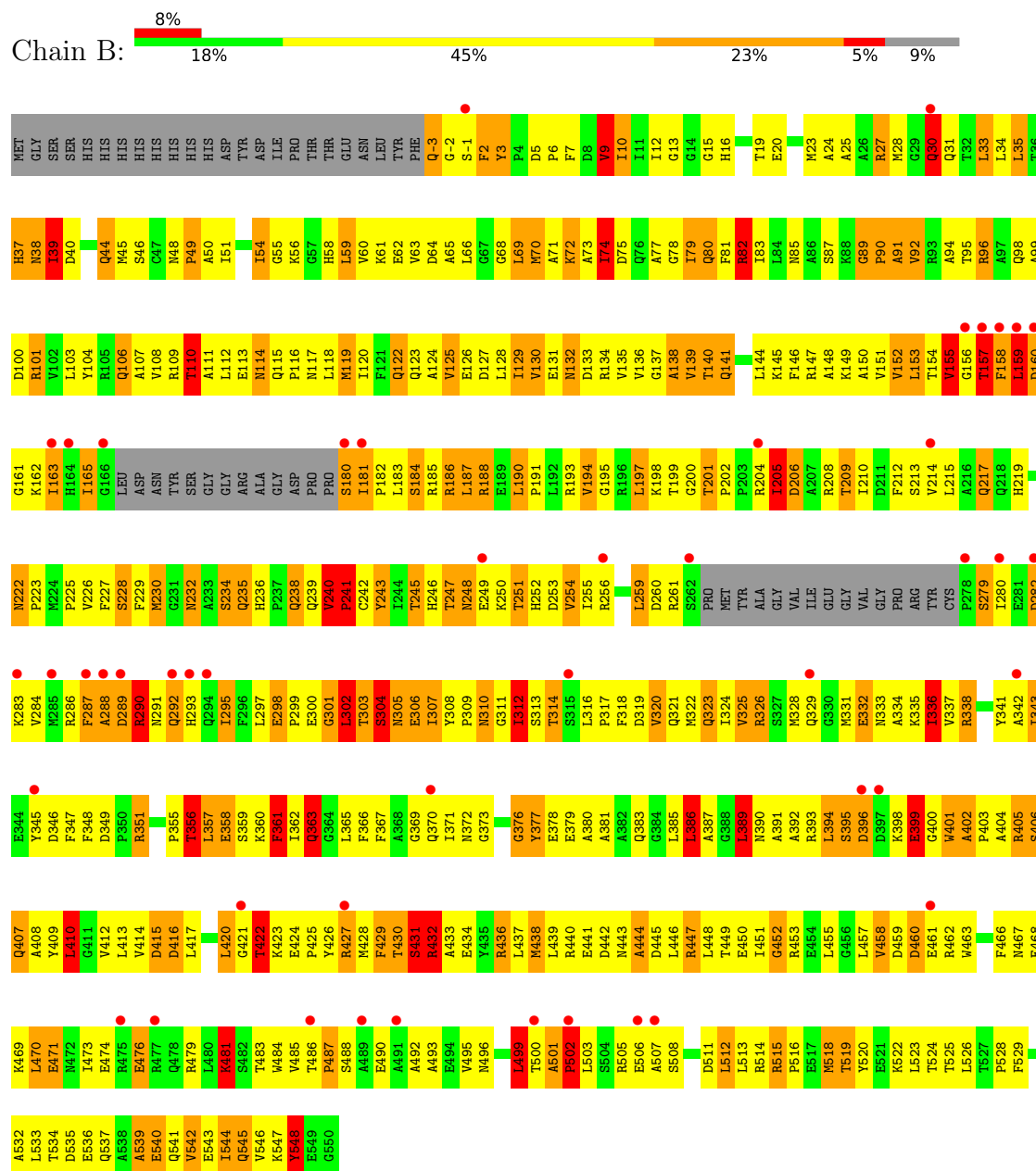
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLN	-	expression tag	UNP Q8XAY0
A	-2	GLY	-	expression tag	UNP Q8XAY0
A	-1	SER	-	expression tag	UNP Q8XAY0
B	-27	MET	-	expression tag	UNP Q8XAY0
B	-26	GLY	-	expression tag	UNP Q8XAY0
B	-25	SER	-	expression tag	UNP Q8XAY0
B	-24	SER	-	expression tag	UNP 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 (CCD ID: SO4) (formula: O₄S).



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

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



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 50.00 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.49) 99.7 (50.00-3.49)	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	Depositor
R, R_{free}	0.227 , 0.265 0.224 , 0.260	Depositor DCC
R_{free} test set	2137 reflections (5.05%)	wwPDB-VP
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 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.06	5/4146 (0.1%)	1.61	80/5615 (1.4%)
1	B	0.96	1/4134 (0.0%)	1.56	74/5596 (1.3%)
All	All	1.01	6/8280 (0.1%)	1.58	154/11211 (1.4%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	ARG	CZ-NH2	23.99	1.64	1.33
1	A	181	ILE	CA-CB	6.67	1.62	1.54
1	A	505	ARG	NE-CZ	5.63	1.39	1.33
1	A	240	VAL	CA-CB	-5.53	1.47	1.54
1	A	125	VAL	CA-CB	-5.21	1.48	1.54
1	B	49	PRO	N-CA	-5.04	1.43	1.47

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ALA	CA-C-N	-13.91	105.39	120.14
1	B	402	ALA	C-N-CA	-13.91	105.39	120.14
1	B	290	ARG	N-CA-C	-13.52	82.01	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	GLN	CA-C-N	12.44	135.39	119.84
1	A	115	GLN	C-N-CA	12.44	135.39	119.84
1	A	201	THR	CB-CA-C	-10.81	93.74	109.63
1	B	152	VAL	CB-CA-C	-10.76	100.42	112.68
1	A	202	PRO	CA-C-N	-10.11	107.20	119.84
1	A	202	PRO	C-N-CA	-10.11	107.20	119.84
1	A	287	PHE	N-CA-C	9.92	121.86	107.88
1	A	402	ALA	CA-C-N	9.39	129.98	119.93
1	A	402	ALA	C-N-CA	9.39	129.98	119.93
1	A	424	GLU	CA-C-N	9.25	129.31	119.78
1	A	424	GLU	C-N-CA	9.25	129.31	119.78
1	A	89	GLY	CA-C-N	9.16	131.29	119.84
1	A	89	GLY	C-N-CA	9.16	131.29	119.84
1	B	205	ILE	N-CA-C	9.01	122.72	108.85
1	B	202	PRO	CA-C-N	-8.76	110.37	119.83
1	B	202	PRO	C-N-CA	-8.76	110.37	119.83
1	A	422	THR	N-CA-C	8.70	122.65	108.55
1	A	314	THR	CB-CA-C	-8.52	94.91	111.78
1	B	444	ALA	N-CA-C	-8.50	102.10	111.36
1	A	298	GLU	CA-C-N	8.43	129.75	119.98
1	A	298	GLU	C-N-CA	8.43	129.75	119.98
1	B	240	VAL	CA-C-N	8.41	130.35	119.84
1	B	240	VAL	C-N-CA	8.41	130.35	119.84
1	B	356	THR	N-CA-C	-8.11	102.85	114.12
1	B	325	VAL	N-CA-C	-8.09	100.98	111.09
1	A	38	ASN	N-CA-C	8.09	120.66	107.32
1	A	290	ARG	N-CA-C	-7.89	100.75	111.87
1	B	113	GLU	CA-C-N	-7.86	110.83	122.86
1	B	113	GLU	C-N-CA	-7.86	110.83	122.86
1	A	28	MET	N-CA-C	-7.71	102.09	112.26
1	A	438	MET	N-CA-C	-7.64	103.41	112.89
1	B	515	ARG	CA-C-N	7.59	129.33	119.84
1	B	515	ARG	C-N-CA	7.59	129.33	119.84
1	B	96	ARG	N-CA-C	7.57	119.82	107.32
1	B	63	VAL	CB-CA-C	-7.54	102.16	112.04
1	A	434	GLU	CB-CA-C	7.36	123.16	110.72
1	A	71	ALA	N-CA-C	-7.27	103.29	111.14
1	A	371	ILE	N-CA-C	-7.23	103.60	113.00
1	A	196	ARG	N-CA-C	-7.16	99.87	110.46
1	A	197	LEU	N-CA-C	-7.09	97.06	108.55
1	B	87	SER	N-CA-C	-7.07	101.96	110.44
1	A	325	VAL	N-CA-C	-7.05	103.98	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	GLU	N-CA-C	7.03	120.85	109.40
1	A	245	THR	N-CA-C	-7.01	99.09	109.81
1	B	101	ARG	NE-CZ-NH1	-7.01	114.49	121.50
1	B	370	GLN	N-CA-C	-6.98	104.84	113.15
1	B	30	GLN	N-CA-C	6.97	119.82	110.35
1	A	501	ALA	CA-C-N	6.94	128.51	119.84
1	A	501	ALA	C-N-CA	6.94	128.51	119.84
1	B	298	GLU	CA-C-N	6.89	128.71	120.23
1	B	298	GLU	C-N-CA	6.89	128.71	120.23
1	A	117	ASN	N-CA-C	6.82	123.98	113.28
1	A	452	GLY	N-CA-C	-6.80	104.26	112.49
1	A	451	ILE	N-CA-C	-6.73	104.25	113.00
1	A	244	ILE	CB-CA-C	-6.71	102.27	110.99
1	A	194	VAL	CB-CA-C	-6.62	101.93	111.34
1	B	248	ASN	N-CA-C	6.56	118.29	107.73
1	B	361	PHE	N-CA-C	6.54	121.46	112.90
1	A	419	THR	N-CA-C	-6.47	103.84	111.03
1	B	501	ALA	CA-C-N	6.47	127.93	119.84
1	B	501	ALA	C-N-CA	6.47	127.93	119.84
1	B	206	ASP	N-CA-C	6.44	118.78	108.41
1	B	410	LEU	N-CA-C	-6.43	103.39	111.11
1	A	505	ARG	NH1-CZ-NH2	-6.42	110.95	119.30
1	B	407	GLN	N-CA-C	-6.42	104.49	112.90
1	B	241	PRO	CB-CA-C	-6.40	101.00	111.56
1	B	129	ILE	N-CA-C	6.38	116.81	107.37
1	A	362	ILE	CB-CA-C	-6.37	101.73	110.77
1	B	332	GLU	N-CA-C	-6.36	103.60	112.45
1	A	337	VAL	N-CA-C	6.36	116.51	110.53
1	A	203	PRO	N-CA-C	-6.27	99.56	112.47
1	B	301	GLY	N-CA-C	6.26	119.45	111.37
1	A	401	TRP	N-CA-C	-6.25	101.03	110.28
1	B	253	ASP	N-CA-C	-6.19	103.46	111.02
1	B	16	HIS	N-CA-C	-6.14	104.51	111.14
1	A	72	LYS	N-CA-C	-6.10	104.33	110.97
1	A	416	ASP	N-CA-C	6.09	118.70	111.33
1	B	108	VAL	N-CA-C	-6.07	103.92	110.23
1	B	458	VAL	N-CA-C	6.05	116.83	108.12
1	B	304	SER	N-CA-C	6.04	118.22	108.32
1	A	315	SER	N-CA-C	-5.98	105.55	114.64
1	A	436	ARG	N-CA-C	-5.92	98.18	110.80
1	A	486	THR	CA-C-N	5.91	127.23	119.84
1	A	486	THR	C-N-CA	5.91	127.23	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	LEU	N-CA-C	5.90	123.37	110.80
1	B	135	VAL	CB-CA-C	-5.87	102.94	111.68
1	A	248	ASN	N-CA-C	5.82	116.09	107.88
1	B	401	TRP	N-CA-C	-5.82	102.15	110.59
1	A	314	THR	N-CA-C	5.81	116.07	107.88
1	B	376	GLY	N-CA-C	5.81	126.95	113.18
1	A	445	ASP	O-C-N	5.79	128.05	122.03
1	B	89	GLY	CA-C-N	5.76	127.05	119.84
1	B	89	GLY	C-N-CA	5.76	127.05	119.84
1	B	356	THR	CB-CA-C	-5.76	99.70	109.38
1	B	140	THR	N-CA-C	-5.73	102.81	110.55
1	B	548	TYR	N-CA-C	5.73	120.07	109.24
1	B	155	VAL	CB-CA-C	-5.73	101.90	111.29
1	B	201	THR	CA-C-N	5.72	123.78	119.66
1	B	201	THR	C-N-CA	5.72	123.78	119.66
1	A	453	ARG	N-CA-C	-5.70	104.27	111.11
1	A	3	TYR	CA-C-N	5.69	126.96	119.84
1	A	3	TYR	C-N-CA	5.69	126.96	119.84
1	A	75	ASP	CB-CA-C	-5.67	101.38	110.79
1	B	34	LEU	CA-C-N	-5.65	114.77	123.14
1	B	34	LEU	C-N-CA	-5.65	114.77	123.14
1	B	130	VAL	CB-CA-C	-5.64	103.35	111.19
1	A	199	THR	N-CA-C	5.62	118.17	110.24
1	A	330	GLY	CA-C-N	-5.58	113.57	122.66
1	A	330	GLY	C-N-CA	-5.58	113.57	122.66
1	B	198	LYS	N-CA-C	5.58	119.62	112.26
1	A	139	VAL	CB-CA-C	-5.56	102.40	110.63
1	A	210	ILE	N-CA-C	5.55	115.89	108.11
1	A	190	LEU	CA-C-N	5.55	126.78	119.84
1	A	190	LEU	C-N-CA	5.55	126.78	119.84
1	B	92	VAL	CB-CA-C	5.55	120.39	111.29
1	B	138	ALA	N-CA-C	5.54	117.05	109.18
1	A	293	HIS	N-CA-C	5.54	118.54	107.62
1	B	6	PRO	CA-C-N	-5.52	114.14	122.81
1	B	6	PRO	C-N-CA	-5.52	114.14	122.81
1	A	299	PRO	CB-CA-C	-5.50	104.56	111.71
1	A	117	ASN	N-CA-CB	-5.49	107.91	114.17
1	B	74	ILE	N-CA-C	-5.45	104.93	112.50
1	A	309	PRO	N-CA-C	-5.43	101.28	112.47
1	B	438	MET	N-CA-C	-5.43	106.33	113.17
1	B	481	LYS	N-CA-C	-5.40	107.24	113.88
1	A	226	VAL	CB-CA-C	-5.36	102.24	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ILE	CA-C-N	-5.36	112.66	121.34
1	B	336	ILE	C-N-CA	-5.36	112.66	121.34
1	B	395	SER	N-CA-C	5.36	118.61	111.75
1	B	396	ASP	N-CA-C	-5.34	106.63	112.72
1	A	-1	SER	N-CA-C	-5.31	104.59	111.71
1	B	422	THR	N-CA-C	-5.29	99.54	110.80
1	A	445	ASP	CA-C-N	5.28	128.74	120.82
1	A	445	ASP	C-N-CA	5.28	128.74	120.82
1	B	429	PHE	CB-CA-C	-5.27	101.98	110.74
1	B	96	ARG	CB-CA-C	-5.27	104.79	111.70
1	A	10	ILE	N-CA-C	5.25	115.66	107.99
1	B	101	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A	135	VAL	CB-CA-C	-5.19	102.78	111.29
1	B	217	GLN	N-CA-C	5.18	116.78	110.41
1	A	198	LYS	N-CA-C	5.16	119.20	108.53
1	A	12	ILE	CB-CA-C	-5.12	104.74	111.25
1	B	544	ILE	CB-CA-C	-5.12	105.16	112.22
1	A	278	PRO	CA-C-N	5.10	128.31	120.82
1	A	278	PRO	C-N-CA	5.10	128.31	120.82
1	A	76	GLN	N-CA-C	-5.09	105.91	111.82
1	A	473	ILE	CB-CA-C	-5.09	105.42	112.24
1	A	251	THR	CB-CA-C	-5.08	102.84	110.92
1	A	122	GLN	N-CA-C	5.06	117.38	107.57
1	A	253	ASP	N-CA-C	-5.01	105.33	111.75
1	B	9	VAL	CB-CA-C	-5.01	103.01	110.33

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
1	B	159	LEU	Peptide
1	B	241	PRO	Peptide

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Mol	Chain	Res	Type	Group
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	592	0
1	B	4063	0	4029	615	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
All	All	8156	0	8055	1204	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 74.

All (1204) 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:285:MET:CA	1:A:285:MET:HE2	1.49	1.42
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:A:289:ASP:C	1:A:291:ASN:HA	1.56	1.30
1:B:154:THR:O	1:B:155:VAL:CG1	1.79	1.29
1:A:285:MET:HA	1:A:285:MET:CE	1.59	1.26
1:A:432:ARG:HB2	1:A:436:ARG:NH1	1.52	1.25
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
1:A:314:THR:HG22	1:A:316:LEU:H	1.05	1.14
1:B:12:ILE:O	1:B:154:THR:HG22	0.97	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:439:LEU:HD23	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:B:154:THR:C	1:B:155:VAL:HG12	1.75	1.09
1:A:284:VAL:O	1:A:286:ARG:N	1.85	1.08
1:A:285:MET:CA	1:A:285:MET:CE	2.25	1.08
1:A:-3:GLN:O	1:A:-3:GLN:HG3	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:262:SER:CB	1:A:263:PRO:CD	2.32	1.06
1:A:404:ALA:CB	1:A:407:GLN:HG3	1.84	1.06
1:B:461:GLU:HG2	1:B:461:GLU:O	1.54	1.06
1:A:289:ASP:CA	1:A:291:ASN:CA	2.33	1.06
1:A:312:ILE:HG21	1:A:328:MET:HE1	1.33	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: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:156:GLY:O	1:B:157:THR:HG23	1.57	1.02
1:B:180:SER:O	1:B:181:ILE:CG2	2.07	1.02
1:B:230:MET:CE	1:B:230:MET:HA	1.89	1.02
1:A:166:GLY:N	1:A:315:SER:O	1.93	1.02
1:A:285:MET:HE2	1:A:285:MET:N	1.73	1.02
1:A:205:ILE:HG21	1:A:210:ILE:HD11	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:SER:OG	1:A:263:PRO:HD2	1.57	1.01
1:A:424:GLU:CD	1:A:436:ARG:HH22	1.67	1.01
1:B:252:HIS:HD2	1:B:284:VAL:HG11	1.26	1.01
1:B:155:VAL:O	1:B:155:VAL:HG22	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:205:ILE:CD1	1:B:336:ILE:HA	1.92	0.99
1:B:209:THR:HG1	1:B:334:ALA:HA	1.19	0.99
1:A:81:PHE:HB3	1:A:225:PRO:HG2	1.43	0.99
1:B:394:LEU:C	1:B:394:LEU:HD23	1.83	0.99
1:A:163:ILE:CG2	1:A:341:TYR:HD2	1.75	0.98
1:A:108:VAL:O	1:A:112:LEU:HD12	1.63	0.98
1:A:448:LEU:CD2	1:A:451:ILE:HD11	1.92	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: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:A:289:ASP:N	1:A:291:ASN:CB	2.28	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:160:ASP:CG	1:B:161:GLY:H	1.73	0.94
1:B:250:LYS:O	1:B:254:VAL:HG23	1.67	0.94
1:A:247:THR:HG22	1:A:293:HIS:H	1.29	0.94
1:A:424:GLU:OE2	1:A:436:ARG:NH2	2.01	0.94
1:B:101:ARG:HH12	1:B:300:GLU:CD	1.75	0.93
1:A:289:ASP:N	1:A:291:ASN:HA	1.83	0.93
1:A:45:MET:HE2	1:A:49:PRO:HA	1.50	0.93
1:B:13:GLY:HA3	1:B:154:THR:HG21	1.47	0.93
1:B:2:PHE:O	1:B:3:TYR:C	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:CG1	1:A:156:GLY:N	2.29	0.92
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:289:ASP:C	1:A:291:ASN:CA	2.44	0.91
1:A:314:THR:CG2	1:A:316:LEU:HB2	2.01	0.91
1:A:203:PRO:HB3	1:A:340:GLY:H	1.34	0.91
1:A:437:LEU:HD12	1:A:437:LEU:O	1.70	0.91
1:A:155:VAL:HG13	1:A:156:GLY:N	1.86	0.90
1:B:158:PHE:O	1:B:159:LEU:C	2.09	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:B:79:ILE:HA	1:B:239:GLN:NE2	1.86	0.90
1:B:217:GLN:NE2	1:B:219:HIS:NE2	2.20	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:A:314:THR:CG2	1:A:316:LEU:H	1.86	0.89
1:A:284:VAL:C	1:A:286:ARG:H	1.79	0.89
1:B:321:GLN:O	1:B:325:VAL:HG23	1.72	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:427:ARG:HH21	1:B:428:MET:HE1	1.37	0.89
1:A:28:MET:HE1	1:A:392:ALA:HB3	1.53	0.88
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:A:432:ARG:CB	1:A:436:ARG:NH1	2.34	0.88
1:A:285:MET:HE2	1:A:285:MET:HA	0.88	0.88
1:A:351:ARG:HD2	1:A:421:GLY:N	1.89	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PHE:HB3	1:B:225:PRO:HG2	1.58	0.84
1:B:37:HIS:ND1	1:B:37:HIS:C	2.36	0.84
1:B:222:ASN:HD22	1:B:223:PRO:HA	1.40	0.84
1:B:476:GLU:O	1:B:476:GLU:HG3	1.75	0.84
1:A:139:VAL:HG13	1:A:145:LYS:HG2	1.58	0.84
1:A:122:GLN:O	1:A:122:GLN:HG2	1.75	0.84
1:A:163:ILE:CG2	1:A:341:TYR:CD2	2.59	0.84
1:B:361:PHE:N	1:B:361:PHE:HD2	1.71	0.84
1:A:440:ARG:HH21	1:A:544:ILE:CG2	1.90	0.84
1:B:181:ILE:HG23	1:B:184:SER:HB2	1.58	0.84
1:A:351:ARG:HD2	1:A:421:GLY:HA3	1.60	0.84
1:A:253:ASP:O	1:A:257:SER:OG	1.95	0.84
1:A:262:SER:HB2	1:A:263:PRO:HD2	1.57	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:81:PHE:CB	1:A:225:PRO:HG2	2.07	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:B:230:MET:HA	1:B:230:MET:HE3	1.60	0.82
1:A:289:ASP:HA	1:A:291:ASN:CB	2.10	0.82
1:B:45:MET:HE3	1:B:104:TYR:CD1	2.15	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:159:LEU:HB3	1:A:160:ASP:CA	2.09	0.81
1:A:289:ASP:CA	1:A:291:ASN:CB	2.58	0.81
1:A:440:ARG:NH2	1:A:544:ILE:HG21	1.94	0.81
1:B:541:GLN:HG3	1:B:545:GLN:HE21	1.45	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:O	1:B:96:ARG:HG2	1.78	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:B:540:GLU:O	1:B:544:ILE:HG12	1.80	0.81
1:A:234:SER:O	1:A:236:HIS:N	2.14	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: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:A:288:ALA:C	1:A:291:ASN:CB	2.54	0.80
1:B:94:ALA:HA	1:B:441:GLU:OE2	1.82	0.79
1:A:424:GLU:CD	1:A:436:ARG:NH2	2.40	0.79
1:B:23:MET:HE1	1:B:115:GLN:OE1	1.82	0.79
1:A:27:ARG:NH2	1:A:67:GLY:C	2.40	0.79
1:A:289:ASP:N	1:A:291:ASN:CA	2.44	0.79
1:B:72:LYS:O	1:B:73:ALA:C	2.25	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:A:382:ALA:HB1	1:A:410:LEU:HD23	1.64	0.78
1:B:541:GLN:HG3	1:B:545:GLN:NE2	1.97	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:158:PHE:O	1:B:158:PHE:CG	2.37	0.77
1:B:209:THR:HG21	1:B:335:LYS:HB2	1.66	0.77
1:B:191:PRO:CG	1:B:361:PHE:CE1	2.67	0.77
1:B:230:MET:HA	1:B:230:MET:HE2	1.67	0.77
1:A:49:PRO:HB3	1:A:101:ARG:NH1	1.99	0.77
1:B:33:LEU:CD2	1:B:35:LEU:HD23	2.15	0.77
1:B:73:ALA:HB1	1:B:104:TYR:CE2	2.18	0.77
1:B:156:GLY:C	1:B:157:THR:CG2	2.57	0.77
1:A:199:THR:O	1:A:343:ILE:HD12	1.85	0.77
1:A:205:ILE:CG2	1:A:210:ILE:HD11	2.14	0.77
1:A:289:ASP:C	1:A:291:ASN:O	2.28	0.77
1:A:385:LEU:HD23	1:A:385:LEU:C	2.09	0.77
1:B:191:PRO:CB	1:B:361:PHE:CE1	2.60	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:139:VAL:CG1	1:A:145:LYS:HG2	2.15	0.76
1:A:156:GLY:O	1:A:157:THR:CG2	2.29	0.76
1:B:101:ARG:NH1	1:B:300:GLU:CD	2.42	0.76
1:A:473:ILE:HG23	1:A:542:VAL:HG23	1.67	0.76
1:B:431:SER:O	1:B:432:ARG:C	2.27	0.76
1:A:439:LEU:HD23	1:A:439:LEU:H	1.46	0.76
1:B:155:VAL:O	1:B:155:VAL:CG2	2.29	0.76
1:B:54:ILE:HD11	1:B:85:ASN:ND2	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLN:HA	1:A:30:GLN:NE2	2.01	0.76
1:B:239:GLN:C	1:B:240:VAL:HG12	2.11	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:B:247:THR:HG23	1:B:248:ASN:N	2.00	0.76
1:A:45:MET:HE1	1:A:49:PRO:HA	1.67	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:A:122:GLN:O	1:A:122:GLN:CG	2.33	0.75
1:B:131:GLU:O	1:B:132:ASN:HB2	1.86	0.75
1:B:356:THR:O	1:B:357:LEU:HB2	1.87	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: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:A:-3:GLN:O	1:A:-2:GLY:C	2.30	0.74
1:A:389:LEU:HD22	1:A:457:LEU:HD11	1.69	0.74
1:B:90:PRO:CB	1:B:440:ARG:HD2	2.14	0.74
1:A:424:GLU:OE1	1:A:436:ARG:NH2	2.20	0.74
1:A:465:ARG:NH1	1:A:535:ASP:OD2	2.17	0.74
1:B:241:PRO:HB2	1:B:243:TYR:HE2	1.52	0.74
1:B:461:GLU:O	1:B:461:GLU:CG	2.35	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:58:HIS:CE1	1:B:429:PHE:CZ	2.75	0.73
1:B:320:VAL:O	1:B:324:ILE:HG13	1.88	0.73
1:A:103:LEU:O	1:A:106:GLN:HB3	1.87	0.73
1:A:389:LEU:HD13	1:A:457:LEU:HD21	1.69	0.73
1:A:284:VAL:C	1:A:286:ARG:N	2.41	0.73
1:B:416:ASP:O	1:B:420:LEU:HD12	1.88	0.73
1:A:200:GLY:HA2	1:A:342:ALA:HA	1.70	0.73
1:A:289:ASP:C	1:A:291:ASN:C	2.56	0.73
1:A:13:GLY:HA3	1:A:154:THR:CG2	2.18	0.73
1:B:394:LEU:C	1:B:394:LEU:CD2	2.61	0.73
1:A:204:ARG:HB2	1:A:338:ARG:HB2	1.71	0.72
1:A:404:ALA:HB3	1:A:407:GLN:CD	2.13	0.72
1:A:129:ILE:HG22	1:A:136:VAL:HG13	1.71	0.72
1:A:404:ALA:CB	1:A:407:GLN:CG	2.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-3:GLN:C	1:B:-1:SER:H	1.96	0.72
1:B:20:GLU:HG3	1:B:381:ALA:HB1	1.71	0.72
1:A:290:ARG:N	1:A:291:ASN:CA	2.36	0.72
1:A:435:TYR:C	1:A:436:ARG:O	2.30	0.72
1:B:389:LEU:HD11	1:B:455:LEU:HD13	1.72	0.72
1:B:27:ARG:HG2	1:B:27:ARG:HH11	1.55	0.72
1:B:12:ILE:C	1:B:154:THR:HG22	2.07	0.72
1:B:190:LEU:HD11	1:B:362:ILE:HD11	1.70	0.72
1:B:155:VAL:O	1:B:155:VAL:HG13	1.87	0.72
1:A:440:ARG:NH2	1:A:544:ILE:CG2	2.51	0.72
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:A:13:GLY:C	1:A:154:THR:HG21	2.13	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:A:413:LEU:HD11	1:A:417:LEU:HD11	1.72	0.71
1:A:432:ARG:HB2	1:A:436:ARG:HH12	1.50	0.71
1:B:292:GLN:HE21	1:B:292:GLN:HA	1.56	0.71
1:B:160:ASP:CG	1:B:161:GLY:N	2.44	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:A:293:HIS:O	1:A:294:GLN:C	2.34	0.71
1:B:389:LEU:HD13	1:B:457:LEU:HD11	1.71	0.71
1:B:405:ARG:O	1:B:405:ARG:HG2	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:A:209:THR:HB	1:A:334:ALA:CA	2.19	0.70
1:B:126:GLU:O	1:B:182:PRO:HG2	1.90	0.70
1:A:165:ILE:C	1:A:166:GLY:O	2.31	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:159:LEU:HB3	1:B:160:ASP:HA	1.73	0.70
1:B:252:HIS:CD2	1:B:284:VAL:CG1	2.71	0.70
1:A:203:PRO:HD2	1:A:203:PRO:O	1.90	0.70
1:A:2:PHE:O	1:A:3:TYR:C	2.32	0.70
1:A:347:PHE:CD1	1:A:347:PHE:C	2.67	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:B:180:SER:C	1:B:181:ILE:HG22	2.14	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASP:HA	1:A:514:ARG:HH21	1.57	0.69
1:B:9:VAL:HG21	1:B:25:ALA:HB1	1.72	0.69
1:A:481:LYS:C	1:A:483:THR:H	2.00	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:468:GLU:O	1:A:472:ASN:HB2	1.92	0.69
1:A:222:ASN:HD22	1:A:223:PRO:HA	1.58	0.69
1:B:470:LEU:O	1:B:473:ILE:N	2.19	0.69
1:A:123:GLN:HG3	1:A:142:MET:HE2	1.75	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
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:61:LYS:HG3	1:B:441:GLU:HG2	1.75	0.68
1:A:473:ILE:HG23	1:A:542:VAL:CG2	2.24	0.68
1:B:467:ASN:O	1:B:470:LEU:N	2.22	0.68
1:A:102:VAL:HG12	1:A:103:LEU:N	2.09	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:38:ASN:C	1:B:40:ASP:H	2.01	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:B:210:ILE:HD13	1:B:331:MET:HE1	1.76	0.67
1:B:222:ASN:HA	1:B:223:PRO:C	2.20	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:33:LEU:HD12	1:A:34:LEU:N	2.10	0.67
1:A:206:ASP:OD1	1:A:208:ARG:HD3	1.95	0.67
1:A:408:ALA:HA	1:A:447:ARG:HH21	1.60	0.66
1:A:28:MET:CE	1:A:392:ALA:HB3	2.24	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:A:115:GLN:O	1:A:115:GLN:HG3	1.95	0.66
1:B:451:ILE:O	1:B:455:LEU:HB2	1.96	0.66
1:A:445:ASP:OD2	1:A:469:LYS:NZ	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ARG:O	1:B:111:ALA:N	2.28	0.66
1:B:230:MET:CE	1:B:230:MET:CA	2.71	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:B:-3:GLN:C	1:B:-1:SER:N	2.53	0.66
1:B:295:ILE:HD11	1:B:311:GLY:O	1.96	0.66
1:B:80:GLN:OE1	1:B:242:CYS:SG	2.54	0.66
1:B:347:PHE:CE1	1:B:373:GLY:HA3	2.31	0.66
1:A:217:GLN:NE2	1:A:219:HIS:NE2	2.44	0.65
1:A:230:MET:HE3	1:A:230:MET:HA	1.78	0.65
1:B:80:GLN:H	1:B:239:GLN:NE2	1.93	0.65
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: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: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:B:292:GLN:HE21	1:B:292:GLN:CA	2.09	0.65
1:B:81:PHE:CZ	1:B:236:HIS:CD2	2.85	0.65
1:B:282:ASP:C	1:B:284:VAL:H	2.04	0.65
1:A:52:GLY:HA2	1:A:56:LYS:HB3	1.78	0.65
1:B:243:TYR:N	1:B:243:TYR:CD2	2.64	0.65
1:B:356:THR:HG22	1:B:390:ASN:OD1	1.96	0.65
1:A:155:VAL:HG12	1:A:156:GLY:H	1.61	0.64
1:A:491:ALA:C	1:A:493:ALA:H	2.02	0.64
1:A:244:ILE:HD13	1:A:296:PHE:CE1	2.32	0.64
1:A:417:LEU:HD23	1:A:417:LEU:N	2.11	0.64
1:B:226:VAL:CG2	1:B:232:ASN:HA	2.26	0.64
1:A:203:PRO:CB	1:A:340:GLY:H	2.06	0.64
1:A:219:HIS:CE1	1:A:241:PRO:HB3	2.32	0.64
1:B:38:ASN:HD22	1:B:40:ASP:H	1.45	0.64
1:B:154:THR:CG2	1:B:155:VAL:N	2.31	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:B:251:THR:O	1:B:255:ILE:HG13	1.97	0.64
1:A:82:ARG:HA	1:A:221:ASP:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PRO:O	1:A:203:PRO:CD	2.44	0.64
1:A:28:MET:HE1	1:A:392:ALA:CB	2.26	0.64
1:A:155:VAL:HG12	1:A:156:GLY:N	2.12	0.64
1:A:405:ARG:HD2	1:A:415:ASP:OD2	1.97	0.64
1:B:247:THR:CG2	1:B:248:ASN:N	2.60	0.64
1:B:109:ARG:O	1:B:110:THR:C	2.41	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: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:314:THR:CG2	1:A:316:LEU:N	2.53	0.63
1:A:432:ARG:O	1:A:434:GLU:N	2.32	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:426:TYR:O	1:B:427:ARG:C	2.40	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:A:45:MET:HE1	1:A:49:PRO:C	2.24	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:B:360:LYS:C	1:B:361:PHE:HD2	2.05	0.63
1:A:166:GLY:CA	1:A:315:SER:O	2.47	0.63
1:A:392:ALA:O	1:A:395:SER:N	2.31	0.63
1:B:195:GLY:HA3	1:B:347:PHE:CE2	2.34	0.63
1:A:28:MET:CE	1:A:392:ALA:CB	2.77	0.62
1:A:430:THR:O	1:A:433:ALA:HB3	1.98	0.62
1:A:491:ALA:C	1:A:493:ALA:N	2.57	0.62
1:B:158:PHE:C	1:B:159:LEU:O	2.40	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:343:ILE:HD12	1:A:343:ILE:N	2.15	0.62
1:A:408:ALA:HB2	1:A:448:LEU:HD11	1.81	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:A:465:ARG:HH12	1:A:535:ASP:CG	2.08	0.62
1:B:38:ASN:C	1:B:40:ASP:N	2.52	0.62
1:B:379:GLU:O	1:B:383:GLN:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:MET:HE2	1:B:230:MET:CA	2.29	0.62
1:B:452:GLY:O	1:B:453:ARG:C	2.43	0.62
1:A:95:THR:HG22	1:A:227:PHE:HE2	1.63	0.62
1:B:54:ILE:HD11	1:B:85:ASN:HD21	1.64	0.62
1:A:209:THR:CB	1:A:334:ALA:HA	2.23	0.62
1:B:126:GLU:HB3	1:B:139:VAL:O	2.00	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:518:MET:HE2	1:B:519:THR:H	1.65	0.61
1:A:289:ASP:HA	1:A:291:ASN:C	2.25	0.61
1:A:108:VAL:O	1:A:112:LEU:CD1	2.46	0.61
1:B:122:GLN:O	1:B:123:GLN:HG2	2.00	0.61
1:A:11:ILE:HG13	1:A:22:ALA:HB2	1.82	0.61
1:B:156:GLY:C	1:B:157:THR:HG22	2.25	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
1:A:312:ILE:HG21	1:A:328:MET:CE	2.19	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:287:PHE:O	1:B:288:ALA:HB2	1.99	0.61
1:B:366:PHE:CD1	1:B:391:ALA:HB2	2.35	0.61
1:A:191:PRO:HG2	1:A:361:PHE:CE2	2.35	0.61
1:A:201:THR:HG22	1:A:202:PRO:CD	2.29	0.61
1:B:7:PHE:N	1:B:147:ARG:O	2.28	0.61
1:B:544:ILE:O	1:B:548:TYR:HD1	1.84	0.61
1:A:37:HIS:NE2	1:A:157:THR:HG23	2.15	0.61
1:A:210:ILE:HG22	1:A:212:PHE:CE2	2.36	0.61
1:A:247:THR:HG22	1:A:293:HIS:N	2.10	0.61
1:A:341:TYR:N	1:A:341:TYR:HD1	1.99	0.61
1:B:62:GLU:HG2	1:B:448:LEU:HD12	1.82	0.61
1:A:285:MET:N	1:A:285:MET:HE3	2.13	0.61
1:A:202:PRO:HA	1:A:313:SER:HA	1.81	0.60
1:B:127:ASP:O	1:B:138:ALA:HB1	2.01	0.60
1:B:290:ARG:HD2	1:B:291:ASN:HD22	1.65	0.60
1:A:45:MET:HE1	1:A:49:PRO:CA	2.30	0.60
1:A:300:GLU:HB2	1:A:306:GLU:O	2.02	0.60
1:A:530:ALA:HB1	1:A:531:PRO:CA	2.30	0.60
1:B:79:ILE:O	1:B:79:ILE:CG1	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:HG21	1:B:341:TYR:CE1	2.36	0.60
1:A:96:ARG:CG	1:A:96:ARG:NH1	2.63	0.60
1:B:163:ILE:H	1:B:163:ILE:HD12	1.66	0.60
1:B:318:PHE:HE1	1:B:336:ILE:HG21	1.65	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: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:A:351:ARG:CD	1:A:421:GLY:CA	2.71	0.60
1:B:492:ALA:O	1:B:496:ASN:ND2	2.35	0.60
1:A:96:ARG:HH11	1:A:96:ARG:HG3	1.66	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:B:486:THR:C	1:B:488:SER:H	2.10	0.60
1:A:153:LEU:HD22	1:A:154:THR:N	2.17	0.60
1:B:380:ALA:O	1:B:381:ALA:C	2.42	0.60
1:B:508:SER:O	1:B:512:LEU:HD23	2.02	0.59
1:A:310:ASN:HD22	1:A:310:ASN:C	2.10	0.59
1:A:393:ARG:HH11	1:A:455:LEU:CD2	2.15	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:A:203:PRO:HB3	1:A:321:GLN:OE1	2.02	0.59
1:A:284:VAL:C	1:A:285:MET:HE2	2.28	0.59
1:A:425:PRO:HB2	1:A:428:MET:HG2	1.83	0.59
1:A:448:LEU:O	1:A:451:ILE:CG1	2.47	0.59
1:B:37:HIS:ND1	1:B:38:ASN:HB2	2.17	0.59
1:A:341:TYR:N	1:A:341:TYR:CD1	2.71	0.59
1:A:408:ALA:O	1:A:411:GLY:N	2.35	0.59
1:B:33:LEU:CD1	1:B:119:MET:HE2	2.33	0.59
1:B:79:ILE:HA	1:B:239:GLN:HE21	1.65	0.59
1:B:306:GLU:CD	1:B:338:ARG:NH1	2.61	0.59
1:A:228:SER:OG	1:A:229:PHE:N	2.34	0.59
1:A:247:THR:CG2	1:A:293:HIS:H	2.09	0.59
1:B:72:LYS:O	1:B:75:ASP:N	2.36	0.59
1:B:154:THR:O	1:B:155:VAL:CB	2.50	0.59
1:A:211:ASP:C	1:A:213:SER:H	2.10	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:72:LYS:O	1:A:73:ALA:C	2.46	0.58
1:A:211:ASP:O	1:A:211:ASP:OD1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:HD13	1:A:541:GLN:NE2	2.18	0.58
1:A:152:VAL:HG22	1:A:366:PHE:HB2	1.84	0.58
1:A:199:THR:HG22	1:A:343:ILE:HD13	1.85	0.58
1:A:349:ASP:OD1	1:A:350:PRO:HD2	2.03	0.58
1:A:351:ARG:HD2	1:A:420:LEU:C	2.27	0.58
1:A:527:THR:N	1:A:528:PRO:CD	2.67	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:A:437:LEU:HD12	1:A:437:LEU:C	2.29	0.58
1:B:191:PRO:HB2	1:B:361:PHE:CZ	2.37	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:B:62:GLU:CD	1:B:408:ALA:HB1	2.28	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:HB2	1:B:188:ARG:HH11	1.66	0.58
1:A:17:ALA:HB2	1:A:380:ALA:HB1	1.85	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:33:LEU:HD12	1:A:33:LEU:C	2.28	0.58
1:B:110:THR:O	1:B:114:ASN:HB2	2.04	0.58
1:B:404:ALA:O	1:B:406:SER:N	2.28	0.58
1:A:230:MET:HA	1:A:230:MET:CE	2.33	0.58
1:A:474:GLU:O	1:A:475:ARG:C	2.46	0.57
1:B:30:GLN:HE21	1:B:30:GLN:N	2.01	0.57
1:B:48:ASN:ND2	1:B:50:ALA:HB3	2.18	0.57
1:B:362:ILE:O	1:B:363:GLN:C	2.47	0.57
1:B:537:GLN:O	1:B:540:GLU:HB3	2.04	0.57
1:B:326:ARG:HH21	1:B:333:ASN:HA	1.69	0.57
1:B:385:LEU:C	1:B:385:LEU:HD23	2.29	0.57
1:B:70:MET:O	1:B:70:MET:HG2	2.03	0.57
1:B:95:THR:N	1:B:441:GLU:OE2	2.37	0.57
1:B:232:ASN:N	1:B:232:ASN:HD22	2.02	0.57
1:A:284:VAL:O	1:A:285:MET:C	2.42	0.57
1:A:354:LYS:C	1:A:356:THR:H	2.11	0.57
1:A:389:LEU:HD21	1:A:455:LEU:HD13	1.86	0.57
1:A:404:ALA:CB	1:A:407:GLN:CD	2.77	0.57
1:A:10:ILE:HG13	1:A:148:ALA:HB2	1.87	0.57
1:A:448:LEU:HD23	1:A:451:ILE:CD1	2.20	0.57
1:B:12:ILE:O	1:B:12:ILE:HG22	2.04	0.57
1:B:243:TYR:N	1:B:243:TYR:HD2	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ILE:HD13	1:B:328:MET:HE1	1.87	0.57
1:B:409:TYR:CZ	1:B:429:PHE:CE1	2.93	0.57
1:A:53:GLY:CA	1:A:96:ARG:HB3	2.35	0.57
1:A:453:ARG:HG2	1:A:463:TRP:CZ2	2.39	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:470:LEU:O	1:B:471:GLU:C	2.47	0.56
1:A:319:ASP:OD2	1:A:319:ASP:N	2.38	0.56
1:B:80:GLN:H	1:B:239:GLN:HE22	1.52	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:A:513:LEU:HD23	1:A:546:VAL:HG11	1.88	0.56
1:B:81:PHE:O	1:B:82:ARG:O	2.23	0.56
1:A:33:LEU:HD12	1:A:119:MET:O	2.05	0.56
1:B:415:ASP:O	1:B:417:LEU:N	2.39	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:B:228:SER:OG	1:B:230:MET:N	2.37	0.56
1:B:415:ASP:O	1:B:416:ASP:C	2.49	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
1:A:127:ASP:HA	1:A:183:LEU:HB2	1.88	0.56
1:B:73:ALA:CB	1:B:104:TYR:CE2	2.89	0.56
1:B:204:ARG:HD2	1:B:338:ARG:HD3	1.88	0.56
1:A:261:ARG:O	1:A:262:SER:O	2.23	0.56
1:B:539:ALA:O	1:B:540:GLU:C	2.49	0.56
1:B:191:PRO:HD2	1:B:361:PHE:CD1	2.41	0.55
1:B:279:SER:HB2	1:B:282:ASP:HB2	1.88	0.55
1:B:306:GLU:OE1	1:B:338:ARG:NH1	2.39	0.55
1:B:427:ARG:NH2	1:B:428:MET:CE	2.68	0.55
1:A:62:GLU:CD	1:A:408:ALA:HB1	2.31	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:B:259:LEU:C	1:B:261:ARG:H	2.14	0.55
1:A:460:ASP:O	1:A:461:GLU:C	2.48	0.55
1:A:185:ARG:O	1:A:186:ARG:C	2.49	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:190:LEU:CB	1:B:191:PRO:CD	2.84	0.55

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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	0.55
1:A:429:PHE:C	1:A:429:PHE:CD2	2.84	0.55
1:A:496:ASN:HD22	1:A:502:PRO:HB3	1.72	0.55
1:B:205:ILE:HD11	1:B:336:ILE:HG13	1.89	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:393:ARG:O	1:B:394:LEU:C	2.50	0.55
1:A:207:ALA:HB2	1:A:305:ASN:O	2.07	0.55
1:B:12:ILE:C	1:B:154:THR:CG2	2.75	0.55
1:B:48:ASN:CB	1:B:308:TYR:CE2	2.83	0.55
1:A:316:LEU:HD13	1:A:320:VAL:HG11	1.89	0.55
1:A:392:ALA:O	1:A:395:SER:OG	2.25	0.55
1:B:181:ILE:HG23	1:B:181:ILE:O	2.07	0.55
1:B:424:GLU:OE2	1:B:436:ARG:NH2	2.36	0.55
1:A:234:SER:C	1:A:236:HIS:H	2.16	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:234:SER:O	1:B:236:HIS:N	2.40	0.54
1:A:38:ASN:ND2	1:A:40:ASP:H	2.04	0.54
1:A:230:MET:HE1	1:A:465:ARG:HG2	1.89	0.54
1:A:471:GLU:O	1:A:472:ASN:C	2.46	0.54
1:B:140:THR:HG21	1:B:146:PHE:HE2	1.71	0.54
1:B:320:VAL:HG12	1:B:324:ILE:HD11	1.89	0.54
1:A:70:MET:CE	1:A:381:ALA:HB2	2.37	0.54
1:A:209:THR:HG21	1:A:335:LYS:HG3	0.83	0.54
1:A:503:LEU:HD21	1:A:512:LEU:HD21	1.88	0.54
1:B:476:GLU:HG2	1:B:533:LEU:HD22	1.88	0.54
1:B:524:THR:HG21	1:B:532:ALA:HA	1.88	0.54
1:B:337:VAL:HG12	1:B:338:ARG:HG3	1.90	0.54
1:A:240:VAL:HG23	1:A:241:PRO:O	2.08	0.54
1:A:440:ARG:NH1	1:A:440:ARG:HG3	2.23	0.54
1:B:162:LYS:O	1:B:343:ILE:HG22	2.06	0.54
1:B:525:THR:HG22	1:B:526:LEU:HD23	1.88	0.54
1:A:278:PRO:CD	1:A:279:SER:H	2.21	0.54
1:A:289:ASP:CA	1:A:291:ASN:C	2.81	0.54
1:A:408:ALA:O	1:A:409:TYR:C	2.49	0.54
1:B:33:LEU:HD12	1:B:119:MET:HG2	1.89	0.54
1:A:379:GLU:OE2	1:A:426:TYR:OH	2.26	0.54
1:A:469:LYS:HE3	1:A:537:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:252:HIS:CD2	1:B:284:VAL:HG13	2.43	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:155:VAL:CG1	1:A:370:GLN:HE21	2.19	0.54
1:A:436:ARG:O	1:A:437:LEU:CB	2.51	0.54
1:A:488:SER:O	1:A:492:ALA:HB2	2.08	0.54
1:A:408:ALA:HA	1:A:447:ARG:NH2	2.21	0.54
1:A:485:VAL:HG23	1:A:503:LEU:CD1	2.38	0.54
1:B:139:VAL:CG1	1:B:145:LYS:HG2	2.19	0.54
1:B:317:PRO:HD2	1:B:320:VAL:HG21	1.90	0.54
1:B:366:PHE:C	1:B:367:PHE:HD1	2.16	0.54
1:B:404:ALA:O	1:B:407:GLN:N	2.28	0.54
1:B:190:LEU:CB	1:B:191:PRO:HD2	2.38	0.54
1:B:372:ASN:HD22	1:B:383:GLN:NE2	2.06	0.54
1:B:371:ILE:HG23	1:B:372:ASN:N	2.22	0.53
1:A:127:ASP:OD1	1:A:186:ARG:NH1	2.42	0.53
1:A:293:HIS:N	1:A:293:HIS:CD2	2.75	0.53
1:A:536:GLU:HA	1:A:536:GLU:OE1	2.07	0.53
1:B:431:SER:C	1:B:433:ALA:N	2.65	0.53
1:A:2:PHE:CE1	1:A:145:LYS:HB3	2.43	0.53
1:A:203:PRO:O	1:A:205:ILE:HD13	2.09	0.53
1:B:71:ALA:O	1:B:72:LYS:C	2.50	0.53
1:B:96:ARG:O	1:B:96:ARG:CG	2.47	0.53
1:B:154:THR:C	1:B:155:VAL:CG1	2.52	0.53
1:B:190:LEU:HB3	1:B:191:PRO:CD	2.39	0.53
1:B:292:GLN:HA	1:B:292:GLN:NE2	2.22	0.53
1:A:484:TRP:CD1	1:A:484:TRP:N	2.76	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:187:LEU:O	1:A:190:LEU:HG	2.09	0.53
1:A:310:ASN:C	1:A:310:ASN:ND2	2.65	0.53
1:A:413:LEU:CD1	1:A:417:LEU:HD11	2.39	0.53
1:B:399:GLU:OE1	1:B:399:GLU:HA	2.09	0.53
1:B:404:ALA:O	1:B:407:GLN:HB2	2.08	0.53
1:A:440:ARG:HG3	1:A:440:ARG:HH11	1.74	0.53
1:A:377:TYR:O	1:A:380:ALA:N	2.40	0.53
1:A:432:ARG:O	1:A:433:ALA:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:LEU:C	1:A:385:LEU:CD2	2.81	0.52
1:A:413:LEU:C	1:A:413:LEU:HD12	2.34	0.52
1:A:30:GLN:NE2	1:A:30:GLN:CA	2.70	0.52
1:A:196:ARG:NH2	1:A:344:GLU:HB3	2.25	0.52
1:A:205:ILE:CG2	1:A:210:ILE:CD1	2.85	0.52
1:A:312:ILE:HD13	1:A:328:MET:HE1	1.91	0.52
1:A:314:THR:CG2	1:A:315:SER:H	2.08	0.52
1:A:519:THR:O	1:A:520:TYR:C	2.52	0.52
1:B:62:GLU:HG2	1:B:448:LEU:CD1	2.38	0.52
1:A:28:MET:HE2	1:A:392:ALA:HB1	1.90	0.52
1:B:318:PHE:HA	1:B:321:GLN:HG3	1.91	0.52
1:A:109:ARG:NH1	1:B:303:THR:O	2.41	0.52
1:A:453:ARG:NH1	1:A:463:TRP:HB2	2.25	0.52
1:B:37:HIS:ND1	1:B:37:HIS:O	2.41	0.52
1:A:11:ILE:HG13	1:A:22:ALA:CA	2.39	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:B:238:GLN:HB3	1:B:302:LEU:HD11	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:B:409:TYR:HA	1:B:412:VAL:HG23	1.92	0.52
1:A:45:MET:HE1	1:A:50:ALA:N	2.25	0.52
1:A:49:PRO:HD2	1:A:298:GLU:OE1	2.09	0.52
1:A:393:ARG:NH1	1:A:455:LEU:CD2	2.73	0.52
1:B:226:VAL:HG12	1:B:227:PHE:N	2.24	0.52
1:B:255:ILE:HG23	1:B:316:LEU:HD11	1.90	0.52
1:A:13:GLY:CA	1:A:154:THR:HG21	2.39	0.52
1:A:289:ASP:O	1:A:291:ASN:O	2.27	0.52
1:B:2:PHE:CE2	1:B:145:LYS:HE3	2.45	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:A:8:ASP:HB3	1:A:395:SER:HB2	1.92	0.51
1:B:385:LEU:HD21	1:B:457:LEU:HD13	1.91	0.51
1:A:16:HIS:O	1:A:17:ALA:C	2.53	0.51
1:A:95:THR:HG21	1:A:227:PHE:CE2	2.46	0.51
1:A:155:VAL:CG1	1:A:156:GLY:H	2.14	0.51
1:A:240:VAL:HG23	1:A:241:PRO:N	2.18	0.51
1:B:322:MET:O	1:B:323:GLN:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:TYR:O	1:B:429:PHE:N	2.40	0.51
1:A:412:VAL:O	1:A:413:LEU:C	2.54	0.51
1:B:357:LEU:O	1:B:358:GLU:C	2.53	0.51
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.43	0.51
1:A:526:LEU:C	1:A:528:PRO:HD2	2.35	0.51
1:B:295:ILE:CD1	1:B:311:GLY:O	2.58	0.51
1:A:24:ALA:O	1:A:25:ALA:C	2.53	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:56:LYS:HD3	1:B:378:GLU:CD	2.36	0.51
1:B:205:ILE:HG23	1:B:206:ASP:H	1.75	0.51
1:B:51:ILE:HD12	1:B:74:ILE:HG12	1.93	0.51
1:B:104:TYR:O	1:B:107:ALA:N	2.34	0.51
1:A:129:ILE:HB	1:A:137:GLY:O	2.11	0.51
1:A:153:LEU:CD2	1:A:154:THR:H	2.23	0.51
1:A:153:LEU:CD2	1:A:154:THR:N	2.74	0.51
1:A:316:LEU:HD13	1:A:320:VAL:CG1	2.41	0.51
1:B:30:GLN:HA	1:B:30:GLN:NE2	2.26	0.51
1:B:358:GLU:N	1:B:366:PHE:CD2	2.79	0.51
1:B:369:GLY:C	1:B:371:ILE:H	2.19	0.51
1:B:30:GLN:NE2	1:B:30:GLN:CA	2.74	0.51
1:A:2:PHE:CE1	1:A:145:LYS:CB	2.94	0.51
1:A:206:ASP:N	1:A:337:VAL:HG23	2.25	0.51
1:A:262:SER:CB	1:A:263:PRO:HD3	2.34	0.51
1:A:377:TYR:O	1:A:378:GLU:C	2.53	0.51
1:B:130:VAL:HG21	1:B:186:ARG:HE	1.76	0.51
1:B:379:GLU:OE1	1:B:379:GLU:N	2.28	0.51
1:A:154:THR:HG23	1:A:155:VAL:N	2.26	0.50
1:A:161:GLY:O	1:A:162:LYS:O	2.29	0.50
1:A:262:SER:OG	1:A:263:PRO:N	2.39	0.50
1:B:56:LYS:O	1:B:60:VAL:HG23	2.11	0.50
1:B:159:LEU:HB3	1:B:160:ASP:CA	2.41	0.50
1:B:437:LEU:O	1:B:437:LEU:HG	2.12	0.50
1:B:459:ASP:C	1:B:461:GLU:N	2.68	0.50
1:A:251:THR:O	1:A:255:ILE:HD12	2.11	0.50
1:B:23:MET:HE3	1:B:23:MET:O	2.11	0.50
1:B:379:GLU:O	1:B:380:ALA:C	2.54	0.50
1:B:422:THR:HG22	1:B:422:THR:O	2.11	0.50
1:B:459:ASP:O	1:B:460:ASP:C	2.54	0.50
1:B:284:VAL:O	1:B:284:VAL:HG12	2.11	0.50
1:B:19:THR:HG23	1:B:112:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:155:VAL:O	1:A:156:GLY:O	2.30	0.50
1:A:199:THR:HG22	1:A:343:ILE:CD1	2.42	0.50
1:A:425:PRO:HD2	1:A:428:MET:HE2	1.93	0.50
1:A:489:ALA:O	1:A:490:GLU:C	2.54	0.50
1:B:156:GLY:O	1:B:157:THR:O	2.30	0.50
1:B:349:ASP:C	1:B:349:ASP:OD1	2.50	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:60:VAL:HG11	1:A:227:PHE:CE1	2.46	0.50
1:A:142:MET:HE3	1:A:144:LEU:HB2	1.94	0.50
1:A:438:MET:C	1:A:439:LEU:HD23	2.33	0.50
1:B:467:ASN:O	1:B:468:GLU:C	2.53	0.50
1:A:90:PRO:HA	1:A:93:ARG:HG3	1.94	0.49
1:A:488:SER:O	1:A:489:ALA:O	2.30	0.49
1:B:459:ASP:O	1:B:462:ARG:N	2.41	0.49
1:B:83:ILE:O	1:B:83:ILE:HG22	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:B:322:MET:O	1:B:326:ARG:HB2	2.13	0.49
1:A:354:LYS:C	1:A:356:THR:N	2.69	0.49
1:B:38:ASN:O	1:B:39:ILE:C	2.52	0.49
1:B:194:VAL:CG2	1:B:348:PHE:HE1	2.24	0.49
1:B:450:GLU:C	1:B:452:GLY:N	2.65	0.49
1:A:479:ARG:HA	1:A:482:SER:HB2	1.95	0.49
1:B:300:GLU:OE2	1:B:308:TYR:HD1	1.96	0.49
1:B:331:MET:N	1:B:332:GLU:OE1	2.45	0.49
1:B:417:LEU:O	1:B:421:GLY:CA	2.53	0.49
1:B:450:GLU:O	1:B:451:ILE:C	2.54	0.49
1:A:165:ILE:O	1:A:166:GLY:O	2.30	0.49
1:A:423:LYS:HE3	1:A:424:GLU:O	2.12	0.49
1:A:378:GLU:OE1	1:A:378:GLU:N	2.43	0.49
1:A:380:ALA:O	1:A:381:ALA:C	2.56	0.49
1:B:19:THR:O	1:B:23:MET:HB2	2.13	0.49
1:B:165:ILE:HG22	1:B:341:TYR:CA	2.41	0.49
1:B:280:ILE:C	1:B:282:ASP:H	2.19	0.49
1:B:366:PHE:CE1	1:B:391:ALA:CB	2.90	0.49
1:A:316:LEU:HD22	1:A:320:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:MET:HE2	1:B:230:MET:O	2.12	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:200:GLY:HA2	1:B:342:ALA:HA	1.95	0.49
1:B:440:ARG:O	1:B:447:ARG:NH1	2.46	0.49
1:A:-3:GLN:O	1:A:-2:GLY:O	2.30	0.48
1:A:314:THR:CG2	1:A:316:LEU:CB	2.84	0.48
1:B:458:VAL:HG13	1:B:462:ARG:HD2	1.94	0.48
1:A:167:LEU:O	1:A:168:ASP:OD1	2.31	0.48
1:A:458:VAL:HG12	1:A:459:ASP:N	2.29	0.48
1:A:469:LYS:HG2	1:A:473:ILE:HD11	1.95	0.48
1:B:205:ILE:HD12	1:B:336:ILE:HA	1.87	0.48
1:A:9:VAL:O	1:A:32:THR:HA	2.12	0.48
1:A:53:GLY:N	1:A:96:ARG:CB	2.77	0.48
1:A:211:ASP:O	1:A:212:PHE:C	2.54	0.48
1:A:430:THR:O	1:A:433:ALA:CB	2.61	0.48
1:B:65:ALA:HB1	1:B:449:THR:OG1	2.13	0.48
1:A:365:LEU:HG	1:A:367:PHE:CE1	2.46	0.48
1:B:188:ARG:HB2	1:B:188:ARG:NH1	2.28	0.48
1:B:194:VAL:CG2	1:B:348:PHE:CD1	2.97	0.48
1:B:520:TYR:HB3	1:B:543:GLU:OE2	2.13	0.48
1:A:463:TRP:O	1:A:466:PHE:HB3	2.13	0.48
1:A:453:ARG:HD2	1:A:453:ARG:HA	1.65	0.48
1:B:363:GLN:HE21	1:B:363:GLN:HB3	1.45	0.48
1:A:45:MET:CE	1:A:49:PRO:CA	2.75	0.48
1:B:371:ILE:HG23	1:B:372:ASN:H	1.79	0.48
1:A:123:GLN:CG	1:A:142:MET:HE2	2.43	0.48
1:A:204:ARG:HD3	1:A:338:ARG:HD2	1.96	0.48
1:A:358:GLU:OE2	1:A:363:GLN:HB3	2.13	0.48
1:B:81:PHE:CZ	1:B:236:HIS:NE2	2.82	0.48
1:B:81:PHE:O	1:B:225:PRO:CG	2.62	0.48
1:B:526:LEU:C	1:B:528:PRO:HD2	2.39	0.48
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:473:ILE:HG23	1:B:542:VAL:HG23	1.95	0.47
1:A:38:ASN:ND2	1:A:38:ASN:C	2.70	0.47
1:A:393:ARG:HH21	1:A:398:LYS:HB3	1.79	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:23:MET:HE2	1:A:69:LEU:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:544:ILE:O	1:A:545:GLN:C	2.55	0.47
1:B:234:SER:O	1:B:235:GLN:C	2.55	0.47
1:A:64:ASP:O	1:A:67:GLY:N	2.39	0.47
1:A:247:THR:O	1:A:248:ASN:HB3	2.14	0.47
1:A:289:ASP:HA	1:A:291:ASN:O	2.13	0.47
1:A:441:GLU:O	1:A:443:ASN:N	2.46	0.47
1:B:128:LEU:HA	1:B:138:ALA:HB2	1.96	0.47
1:A:34:LEU:C	1:A:34:LEU:HD12	2.39	0.47
1:A:41:THR:O	1:A:42:LEU:C	2.58	0.47
1:A:444:ALA:O	1:A:448:LEU:HB2	2.14	0.47
1:A:11:ILE:HD12	1:A:21:ALA:CB	2.44	0.47
1:A:153:LEU:HD22	1:A:154:THR:H	1.78	0.47
1:B:165:ILE:HG23	1:B:341:TYR:HB2	1.96	0.47
1:B:183:LEU:O	1:B:183:LEU:HG	2.14	0.47
1:B:239:GLN:O	1:B:240:VAL:HG12	2.14	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:A:89:GLY:CA	1:A:93:ARG:HE	2.28	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:413:LEU:O	1:B:414:VAL:C	2.58	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: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:385:LEU:HD23	1:B:385:LEU:O	2.15	0.46
1:B:51:ILE:HB	1:B:74:ILE:HG13	1.97	0.46
1:B:65:ALA:HA	1:B:462:ARG:NH1	2.29	0.46
1:B:222:ASN:C	1:B:223:PRO:O	2.55	0.46
1:A:11:ILE:HG13	1:A:22:ALA:CB	2.45	0.46
1:B:48:ASN:HA	1:B:49:PRO:HD3	1.66	0.46
1:B:80:GLN:H	1:B:239:GLN:CD	2.24	0.46
1:B:197:LEU:HD12	1:B:345:TYR:CB	2.41	0.46
1:B:518:MET:SD	1:B:523:LEU:HD12	2.55	0.46
1:B:91:ALA:H	1:B:440:ARG:HD2	1.80	0.46
1:B:106:GLN:O	1:B:106:GLN:HG3	2.12	0.46
1:B:428:MET:O	1:B:429:PHE:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:O	1:A:117:ASN:HB2	2.15	0.46
1:B:115:GLN:O	1:B:116:PRO:C	2.56	0.46
1:B:228:SER:OG	1:B:229:PHE:N	2.45	0.46
1:B:409:TYR:CE1	1:B:439:LEU:HB3	2.50	0.46
1:A:410:LEU:HD13	1:A:410:LEU:O	2.15	0.46
1:A:423:LYS:HE2	1:A:426:TYR:CE2	2.51	0.46
1:A:81:PHE:HB3	1:A:225:PRO:CG	2.29	0.46
1:A:219:HIS:ND1	1:A:241:PRO:HB3	2.30	0.46
1:A:463:TRP:HA	1:A:463:TRP:CE3	2.50	0.46
1:B:64:ASP:OD1	1:B:228:SER:HB2	2.15	0.46
1:A:294:GLN:HE21	1:A:294:GLN:HB2	1.58	0.46
1:A:295:ILE:CD1	1:A:312:ILE:HG23	2.45	0.46
1:A:423:LYS:HG2	1:A:424:GLU:O	2.16	0.46
1:B:13:GLY:CA	1:B:154:THR:CG2	2.77	0.46
1:B:292:GLN:CA	1:B:292:GLN:NE2	2.75	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:348:PHE:N	1:B:371:ILE:O	2.49	0.46
1:B:357:LEU:HD23	1:B:357:LEU:HA	1.77	0.46
1:A:393:ARG:NH2	1:A:398:LYS:HB3	2.30	0.46
1:B:2:PHE:HE2	1:B:145:LYS:HE3	1.82	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:B:290:ARG:HD2	1:B:291:ASN:ND2	2.28	0.46
1:B:301:GLY:O	1:B:303:THR:N	2.49	0.46
1:B:444:ALA:HA	1:B:447:ARG:NH1	2.31	0.46
1:A:338:ARG:NH2	1:B:39:ILE:HB	2.12	0.45
1:A:481:LYS:HD3	1:A:481:LYS:N	2.32	0.45
1:A:466:PHE:CD1	1:A:466:PHE:C	2.94	0.45
1:B:38:ASN:C	1:B:38:ASN:HD22	2.25	0.45
1:A:186:ARG:HH11	1:A:186:ARG:CB	2.30	0.45
1:A:426:TYR:O	1:A:427:ARG:C	2.60	0.45
1:B:158:PHE:O	1:B:158:PHE:CD1	2.68	0.45
1:B:295:ILE:HD13	1:B:295:ILE:HA	1.62	0.45
1:A:259:LEU:C	1:A:261:ARG:H	2.24	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:A:370:GLN:C	1:A:372:ASN:N	2.70	0.45
1:B:77:ALA:O	1:B:99:ALA:HA	2.17	0.45
1:B:215:LEU:CD2	1:B:329:GLN:HG2	2.46	0.45
1:A:208:ARG:O	1:A:210:ILE:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ARG:O	1:B:507:ALA:N	2.50	0.45
1:A:248:ASN:O	1:A:249:GLU:C	2.60	0.45
1:A:484:TRP:HA	1:A:508:SER:HA	1.98	0.45
1:B:367:PHE:N	1:B:367:PHE:CD1	2.84	0.45
1:B:416:ASP:OD1	1:B:420:LEU:HD11	2.17	0.45
1:B:427:ARG:NH2	1:B:428:MET:HE2	2.31	0.45
1:B:445:ASP:O	1:B:449:THR:HB	2.16	0.45
1:A:7:PHE:CD2	1:A:33:LEU:HB2	2.52	0.45
1:A:9:VAL:HG22	1:A:150:ALA:HB3	1.99	0.45
1:A:92:VAL:HG21	1:A:430:THR:HG23	1.99	0.45
1:A:186:ARG:O	1:A:187:LEU:C	2.58	0.45
1:A:287:PHE:HB3	1:A:288:ALA:O	2.16	0.45
1:A:440:ARG:NH2	1:A:544:ILE:HG22	2.30	0.45
1:B:9:VAL:HA	1:B:150:ALA:O	2.16	0.45
1:B:31:GLN:HA	1:B:31:GLN:HE21	1.77	0.45
1:B:44:GLN:HE21	1:B:44:GLN:HB2	1.55	0.45
1:B:64:ASP:OD2	1:B:462:ARG:NH1	2.46	0.45
1:B:116:PRO:O	1:B:117:ASN:HB2	2.17	0.45
1:B:386:LEU:O	1:B:389:LEU:HB3	2.17	0.45
1:B:396:ASP:CG	1:B:398:LYS:HE3	2.41	0.45
1:A:37:HIS:CD2	1:A:157:THR:HG23	2.52	0.45
1:A:53:GLY:HA2	1:A:96:ARG:HB3	1.99	0.45
1:A:208:ARG:C	1:A:210:ILE:H	2.25	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: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:A:166:GLY:CA	1:A:317:PRO:HG3	2.33	0.44
1:A:372:ASN:ND2	1:A:383:GLN:HE21	2.08	0.44
1:A:467:ASN:HA	1:A:470:LEU:HB3	1.99	0.44
1:A:474:GLU:HB3	1:A:475:ARG:H	1.57	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:B:98:GLN:HE22	1:B:298:GLU:CD	2.24	0.44
1:B:100:ASP:O	1:B:101:ARG:C	2.60	0.44
1:B:124:ALA:HB3	1:B:141:GLN:HB3	1.99	0.44
1:B:206:ASP:HB3	1:B:209:THR:CG2	2.46	0.44
1:B:371:ILE:CG2	1:B:372:ASN:H	2.29	0.44
1:B:390:ASN:HD22	1:B:390:ASN:HA	1.41	0.44
1:A:52:GLY:N	1:A:378:GLU:OE2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:O	1:A:110:THR:C	2.60	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:303:THR:O	1:B:303:THR:OG1	2.36	0.44
1:A:11:ILE:HG21	1:A:18:GLY:O	2.17	0.44
1:A:59:LEU:HD12	1:A:59:LEU:HA	1.87	0.44
1:A:443:ASN:OD1	1:A:443:ASN:C	2.59	0.44
1:A:535:ASP:OD1	1:A:535:ASP:C	2.61	0.44
1:B:184:SER:O	1:B:185:ARG:C	2.59	0.44
1:B:495:VAL:HG11	1:B:503:LEU:HD11	1.99	0.44
1:A:80:GLN:HE21	1:A:98:GLN:HG2	1.82	0.44
1:A:123:GLN:HG3	1:A:142:MET:CE	2.45	0.44
1:A:202:PRO:CA	1:A:313:SER:HA	2.46	0.44
1:A:215:LEU:N	1:A:215:LEU:HD23	2.32	0.44
1:A:396:ASP:OD1	1:A:396:ASP:O	2.35	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:481:LYS:C	1:B:483:THR:H	2.26	0.44
1:B:484:TRP:HA	1:B:508:SER:HA	1.98	0.44
1:A:84:LEU:N	1:A:94:ALA:O	2.51	0.44
1:B:213:SER:C	1:B:215:LEU:H	2.25	0.44
1:B:500:THR:HG23	1:B:501:ALA:N	2.32	0.44
1:A:232:ASN:N	1:A:235:GLN:OE1	2.44	0.44
1:B:81:PHE:HB3	1:B:225:PRO:HD2	2.00	0.44
1:B:282:ASP:C	1:B:284:VAL:N	2.67	0.44
1:A:207:ALA:CB	1:A:305:ASN:O	2.66	0.44
1:A:441:GLU:C	1:A:443:ASN:H	2.25	0.44
1:B:28:MET:CE	1:B:392:ALA:HB3	2.47	0.44
1:B:81:PHE:O	1:B:82:ARG:C	2.57	0.44
1:B:137:GLY:HA3	1:B:146:PHE:O	2.18	0.44
1:B:405:ARG:HG3	1:B:412:VAL:HA	2.00	0.44
1:B:495:VAL:O	1:B:499:LEU:HD23	2.18	0.44
1:A:27:ARG:HH22	1:A:68:GLY:N	2.15	0.44
1:A:41:THR:OG1	1:A:157:THR:OG1	2.34	0.44
1:B:496:ASN:HB3	1:B:502:PRO:HB3	2.00	0.44
1:A:27:ARG:NH2	1:A:68:GLY:N	2.65	0.44
1:A:202:PRO:HG3	1:A:308:TYR:CE2	2.53	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:B:109:ARG:C	1:B:111:ALA:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLN:O	1:B:141:GLN:HG2	2.17	0.44
1:B:191:PRO:CD	1:B:361:PHE:CE1	3.00	0.44
1:B:209:THR:OG1	1:B:334:ALA:CA	2.44	0.44
1:B:290:ARG:CD	1:B:291:ASN:HD22	2.31	0.44
1:B:396:ASP:OD1	1:B:396:ASP:O	2.36	0.44
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:B:130:VAL:HG21	1:B:186:ARG:NE	2.32	0.43
1:A:2:PHE:CD1	1:A:145:LYS:CB	2.98	0.43
1:A:38:ASN:O	1:A:39:ILE:C	2.59	0.43
1:A:69:LEU:O	1:A:70:MET:C	2.61	0.43
1:A:289:ASP:CA	1:A:291:ASN:O	2.65	0.43
1:A:477:ARG:HG3	1:A:477:ARG:HH11	1.83	0.43
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.64	0.43
1:B:64:ASP:CG	1:B:462:ARG:HH22	2.23	0.43
1:B:300:GLU:OE2	1:B:308:TYR:CD1	2.71	0.43
1:B:399:GLU:OE1	1:B:399:GLU:CA	2.66	0.43
1:B:459:ASP:C	1:B:461:GLU:H	2.25	0.43
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.58	0.43
1:A:317:PRO:HD2	1:A:320:VAL:HG21	2.00	0.43
1:A:403:PRO:HG2	1:A:410:LEU:HD12	2.00	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:B:245:THR:HG23	1:B:246:HIS:N	2.33	0.43
1:B:366:PHE:HD1	1:B:366:PHE:H	1.66	0.43
1:A:310:ASN:HD22	1:A:311:GLY:N	2.15	0.43
1:B:7:PHE:O	1:B:148:ALA:CA	2.61	0.43
1:A:479:ARG:HG2	1:A:479:ARG:O	2.19	0.43
1:B:195:GLY:O	1:B:346:ASP:HA	2.19	0.43
1:B:476:GLU:O	1:B:476:GLU:CD	2.61	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:A:413:LEU:CD1	1:A:417:LEU:HD21	2.49	0.43
1:A:425:PRO:HD2	1:A:428:MET:CE	2.49	0.43
1:B:115:GLN:O	1:B:115:GLN:HG3	2.19	0.43
1:B:248:ASN:O	1:B:249:GLU:C	2.62	0.43
1:B:367:PHE:HD1	1:B:367:PHE:N	2.17	0.43
1:B:371:ILE:CG2	1:B:372:ASN:N	2.82	0.43
1:B:401:TRP:CD1	1:B:402:ALA:H	2.37	0.43
1:A:100:ASP:OD1	1:A:100:ASP:C	2.61	0.43
1:A:166:GLY:HA2	1:A:315:SER:O	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLY:C	1:A:331:MET:HE2	2.43	0.43
1:A:481:LYS:C	1:A:483:THR:N	2.67	0.43
1:A:541:GLN:O	1:A:542:VAL:C	2.62	0.43
1:B:139:VAL:HG13	1:B:145:LYS:CD	2.47	0.43
1:B:204:ARG:O	1:B:205:ILE:HD13	2.18	0.43
1:A:80:GLN:O	1:A:97:ALA:HA	2.19	0.43
1:A:81:PHE:CZ	1:A:236:HIS:CE1	3.07	0.43
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:537:GLN:O	1:A:538:ALA:C	2.62	0.43
1:A:56:LYS:HB3	1:A:378:GLU:HG2	2.01	0.43
1:A:70:MET:HE3	1:A:381:ALA:HB2	2.01	0.43
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.52	0.43
1:A:212:PHE:HD1	1:A:243:TYR:CD2	2.37	0.43
1:A:366:PHE:C	1:A:367:PHE:HD1	2.27	0.43
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.87	0.43
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.63	0.43
1:B:118:LEU:HD12	1:B:119:MET:N	2.34	0.43
1:A:413:LEU:HD13	1:A:417:LEU:HD21	2.01	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:B:423:LYS:HG2	1:B:424:GLU:N	2.34	0.43
1:A:70:MET:HE1	1:A:381:ALA:HB2	2.01	0.42
1:B:79:ILE:CA	1:B:239:GLN:NE2	2.71	0.42
1:A:259:LEU:C	1:A:261:ARG:N	2.77	0.42
1:A:519:THR:O	1:A:522:LYS:N	2.52	0.42
1:B:302:LEU:HA	1:B:302:LEU:HD23	1.50	0.42
1:A:31:GLN:OE1	1:A:117:ASN:ND2	2.52	0.42
1:B:222:ASN:CA	1:B:223:PRO:C	2.88	0.42
1:B:409:TYR:OH	1:B:429:PHE:CE1	2.70	0.42
1:B:423:LYS:HB3	1:B:423:LYS:HE3	1.80	0.42
1:B:448:LEU:HA	1:B:448:LEU:HD23	1.77	0.42
1:A:7:PHE:CD1	1:A:7:PHE:N	2.87	0.42
1:A:354:LYS:O	1:A:356:THR:N	2.52	0.42
1:A:429:PHE:CD2	1:A:429:PHE:O	2.72	0.42
1:A:490:GLU:OE2	1:A:490:GLU:HA	2.19	0.42
1:B:98:GLN:HE22	1:B:298:GLU:CG	2.30	0.42
1:B:386:LEU:HB3	1:B:387:ALA:H	1.70	0.42
1:A:508:SER:O	1:A:509:GLY:C	2.61	0.42
1:B:38:ASN:ND2	1:B:40:ASP:H	2.15	0.42
1:B:100:ASP:OD2	1:B:302:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:299:PRO:O	1:B:299:PRO:HG2	2.18	0.42
1:B:485:VAL:HG11	1:B:528:PRO:HG3	2.02	0.42
1:A:95:THR:HG21	1:A:227:PHE:CD2	2.54	0.42
1:B:-1:SER:OG	1:B:-1:SER:O	2.36	0.42
1:B:126:GLU:OE1	1:B:126:GLU:HA	2.20	0.42
1:B:181:ILE:HA	1:B:182:PRO:HD2	1.79	0.42
1:B:493:ALA:HA	1:B:496:ASN:HD22	1.84	0.42
1:B:539:ALA:O	1:B:541:GLN:N	2.52	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:242:CYS:HB3	1:B:297:LEU:O	2.19	0.42
1:B:305:ASN:N	1:B:305:ASN:OD1	2.48	0.42
1:B:365:LEU:CD2	1:B:367:PHE:HE1	2.32	0.42
1:B:439:LEU:HD23	1:B:439:LEU:HA	1.45	0.42
1:A:463:TRP:HA	1:A:463:TRP:HE3	1.85	0.42
1:B:131:GLU:N	1:B:134:ARG:O	2.53	0.42
1:B:190:LEU:N	1:B:190:LEU:HD23	2.35	0.42
1:B:304:SER:C	1:B:306:GLU:H	2.28	0.42
1:B:314:THR:HG23	1:B:316:LEU:CA	2.49	0.42
1:A:31:GLN:OE1	1:A:31:GLN:HA	2.19	0.42
1:A:428:MET:SD	1:A:432:ARG:NH2	2.93	0.42
1:B:356:THR:C	1:B:357:LEU:HG	2.44	0.42
1:B:486:THR:C	1:B:488:SER:N	2.77	0.42
1:A:27:ARG:NH2	1:A:67:GLY:CA	2.83	0.42
1:A:393:ARG:HH11	1:A:455:LEU:HD23	1.83	0.42
1:B:316:LEU:HD22	1:B:320:VAL:HG11	2.02	0.42
1:B:446:LEU:HD23	1:B:446:LEU:HA	1.89	0.42
1:B:79:ILE:O	1:B:79:ILE:HG13	2.20	0.41
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:A:12:ILE:HD13	1:A:12:ILE:HG23	1.84	0.41
1:A:57:GLY:O	1:A:60:VAL:N	2.51	0.41
1:A:317:PRO:O	1:A:321:GLN:HG3	2.19	0.41
1:A:331:MET:HE2	1:A:331:MET:N	2.35	0.41
1:B:431:SER:C	1:B:433:ALA:H	2.27	0.41
1:B:508:SER:O	1:B:511:ASP:HB2	2.20	0.41
1:A:7:PHE:CE2	1:A:33:LEU:HB2	2.55	0.41
1:A:25:ALA:O	1:A:30:GLN:HB2	2.21	0.41
1:A:127:ASP:OD1	1:A:128:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASP:C	1:A:284:VAL:N	2.78	0.41
1:A:282:ASP:C	1:A:284:VAL:H	2.28	0.41
1:A:428:MET:O	1:A:429:PHE:C	2.62	0.41
1:A:525:THR:HG23	1:A:525:THR:O	2.19	0.41
1:B:250:LYS:O	1:B:251:THR:C	2.62	0.41
1:B:414:VAL:O	1:B:415:ASP:C	2.60	0.41
1:A:106:GLN:O	1:A:109:ARG:N	2.54	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:425:PRO:HB2	1:B:428:MET:HG2	2.01	0.41
1:B:450:GLU:HB3	1:B:463:TRP:CH2	2.56	0.41
1:B:487:PRO:HB3	1:B:503:LEU:O	2.20	0.41
1:B:524:THR:CG2	1:B:532:ALA:HA	2.51	0.41
1:A:295:ILE:HD13	1:A:295:ILE:HA	1.92	0.41
1:A:443:ASN:O	1:A:446:LEU:HB2	2.21	0.41
1:B:33:LEU:HD12	1:B:119:MET:HE2	2.03	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:A:280:ILE:C	1:A:282:ASP:N	2.76	0.41
1:A:307:ILE:HD12	1:A:307:ILE:HA	1.72	0.41
1:B:434:GLU:O	1:B:437:LEU:HB2	2.20	0.41
1:A:81:PHE:HB2	1:A:225:PRO:HG2	1.98	0.41
1:A:129:ILE:N	1:A:137:GLY:O	2.42	0.41
1:A:167:LEU:H	1:A:167:LEU:HG	1.39	0.41
1:A:230:MET:HB3	1:A:230:MET:HE2	1.79	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:512:LEU:HD12	1:A:529:PHE:HE2	1.85	0.41
1:B:24:ALA:HA	1:B:27:ARG:HG2	2.02	0.41
1:B:449:THR:O	1:B:449:THR:CG2	2.69	0.41
1:B:515:ARG:HA	1:B:516:PRO:HD3	1.93	0.41
1:A:224:MET:HA	1:A:225:PRO:HD2	1.62	0.41
1:B:297:LEU:CD1	1:B:331:MET:HE1	2.51	0.41
1:B:310:ASN:HD22	1:B:310:ASN:C	2.24	0.41
1:B:362:ILE:O	1:B:363:GLN:O	2.38	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:A:100:ASP:O	1:A:101:ARG:C	2.64	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:A:396:ASP:O	1:A:396:ASP:CG	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:358:GLU:O	1:B:359:SER:C	2.63	0.41
1:B:390:ASN:HD21	1:B:401:TRP:H	1.67	0.41
1:B:436:ARG:O	1:B:438:MET:N	2.48	0.41
1:B:446:LEU:HA	1:B:466:PHE:HZ	1.86	0.41
1:B:518:MET:HE2	1:B:519:THR:N	2.33	0.41
1:A:11:ILE:HD12	1:A:21:ALA:HB3	2.03	0.41
1:A:28:MET:HE2	1:A:392:ALA:CB	2.49	0.41
1:A:120:ILE:HG22	1:A:121:PHE:N	2.36	0.41
1:A:203:PRO:HA	1:A:340:GLY:N	2.35	0.41
1:A:289:ASP:H	1:A:291:ASN:HA	1.80	0.41
1:A:392:ALA:O	1:A:395:SER:CB	2.69	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:B:386:LEU:HD22	1:B:410:LEU:HD11	2.03	0.41
1:A:90:PRO:HG2	1:A:548:TYR:CD1	2.56	0.40
1:A:159:LEU:CB	1:A:160:ASP:CA	2.92	0.40
1:A:206:ASP:OD1	1:A:208:ARG:N	2.49	0.40
1:B:331:MET:HE2	1:B:331:MET:HB3	1.86	0.40
1:B:417:LEU:HD23	1:B:422:THR:H	1.86	0.40
1:A:378:GLU:H	1:A:378:GLU:CD	2.29	0.40
1:A:115:GLN:HA	1:A:116:PRO:HD2	1.08	0.40
1:A:166:GLY:O	1:A:168:ASP:N	2.54	0.40
1:A:460:ASP:C	1:A:462:ARG:N	2.76	0.40
1:B:55:GLY:O	1:B:56:LYS:C	2.64	0.40
1:B:70:MET:HE1	1:B:377:TYR:O	2.21	0.40
1:B:392:ALA:O	1:B:395:SER:OG	2.38	0.40
1:A:202:PRO:HB2	1:A:203:PRO:CD	2.51	0.40
1:A:212:PHE:H	1:A:212:PHE:HD2	1.67	0.40
1:A:419:THR:HB	1:A:420:LEU:HG	2.02	0.40
1:B:210:ILE:CD1	1:B:331:MET:CE	2.99	0.40
1:B:222:ASN:CA	1:B:223:PRO:O	2.69	0.40
1:B:322:MET:HE2	1:B:326:ARG:HH12	1.86	0.40
1:A:232:ASN:O	1:A:235:GLN:HB2	2.22	0.40
1:A:316:LEU:HA	1:A:316:LEU:HD23	1.91	0.40
1:B:81:PHE:C	1:B:82:ARG:O	2.65	0.40
1:B:152:VAL:O	1:B:153:LEU:C	2.65	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/576 (90%)	383 (74%)	88 (17%)	50 (10%)	0	6
1	B	518/576 (90%)	363 (70%)	98 (19%)	57 (11%)	0	5
All	All	1039/1152 (90%)	746 (72%)	186 (18%)	107 (10%)	0	5

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	324 (76%)	102 (24%)	1	4
1	B	427/474 (90%)	310 (73%)	117 (27%)	0	3
All	All	853/948 (90%)	634 (74%)	219 (26%)	0	3

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	2	PHE
1	A	5	ASP
1	A	12	ILE
1	A	30	GLN
1	A	39	ILE
1	A	44	GLN
1	A	49	PRO
1	A	51	ILE
1	A	54	ILE
1	A	66	LEU
1	A	69	LEU
1	A	70	MET
1	A	74	ILE
1	A	76	GLN
1	A	79	ILE
1	A	82	ARG
1	A	92	VAL
1	A	93	ARG
1	A	96	ARG
1	A	100	ASP
1	A	102	VAL
1	A	106	GLN
1	A	110	THR
1	A	115	GLN
1	A	125	VAL
1	A	136	VAL

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Mol	Chain	Res	Type
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	205	ILE
1	A	208	ARG
1	A	209	THR
1	A	214	VAL
1	A	217	GLN
1	A	230	MET
1	A	240	VAL
1	A	244	ILE
1	A	245	THR
1	A	251	THR
1	A	257	SER
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	293	HIS
1	A	294	GLN
1	A	295	ILE
1	A	302	LEU
1	A	307	ILE
1	A	313	SER
1	A	319	ASP
1	A	322	MET
1	A	327	SER
1	A	331	MET
1	A	341	TYR
1	A	343	ILE
1	A	351	ARG
1	A	354	LYS
1	A	363	GLN

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Mol	Chain	Res	Type
1	A	370	GLN
1	A	371	ILE
1	A	383	GLN
1	A	394	LEU
1	A	397	ASP
1	A	413	LEU
1	A	414	VAL
1	A	417	LEU
1	A	422	THR
1	A	425	PRO
1	A	428	MET
1	A	431	SER
1	A	432	ARG
1	A	434	GLU
1	A	437	LEU
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	499	LEU
1	A	502	PRO
1	A	504	SER
1	A	527	THR
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	10	ILE
1	B	27	ARG
1	B	30	GLN
1	B	33	LEU
1	B	35	LEU
1	B	37	HIS

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Mol	Chain	Res	Type
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	125	VAL
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	159	LEU
1	B	163	ILE
1	B	165	ILE
1	B	180	SER
1	B	184	SER
1	B	186	ARG
1	B	187	LEU
1	B	188	ARG
1	B	190	LEU
1	B	193	ARG
1	B	194	VAL
1	B	197	LEU
1	B	199	THR
1	B	205	ILE
1	B	208	ARG
1	B	209	THR
1	B	214	VAL
1	B	222	ASN

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Mol	Chain	Res	Type
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	302	LEU
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	320	VAL
1	B	323	GLN
1	B	326	ARG
1	B	336	ILE
1	B	338	ARG
1	B	343	ILE
1	B	351	ARG
1	B	355	PRO
1	B	356	THR
1	B	361	PHE
1	B	363	GLN
1	B	377	TYR
1	B	386	LEU
1	B	389	LEU
1	B	399	GLU

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Mol	Chain	Res	Type
1	B	410	LEU
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	479	ARG
1	B	481	LYS
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	545	GLN
1	B	546	VAL
1	B	547	LYS
1	B	548	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) 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	85	ASN
1	A	117	ASN
1	A	217	GLN
1	A	218	GLN
1	A	222	ASN
1	A	252	HIS
1	A	294	GLN
1	A	310	ASN
1	A	329	GLN
1	A	363	GLN

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Mol	Chain	Res	Type
1	A	370	GLN
1	A	383	GLN
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	235	GLN
1	B	236	HIS
1	B	239	GLN
1	B	246	HIS
1	B	252	HIS
1	B	291	ASN
1	B	292	GLN
1	B	294	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	551	-	4,4,4	0.31	0	6,6,6	0.33	0
2	SO4	B	1	-	4,4,4	0.31	0	6,6,6	0.56	0
2	SO4	A	552	-	4,4,4	0.27	0	6,6,6	0.60	0
2	SO4	A	551	-	4,4,4	0.25	0	6,6,6	0.51	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%)	0.53	47 (8%)	15 10	53, 73, 123, 136	0
1	B	524/576 (90%)	0.55	47 (8%)	15 10	55, 79, 130, 137	0
All	All	1051/1152 (91%)	0.54	94 (8%)	15 10	53, 75, 128, 137	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	PRO	8.3
1	A	181	ILE	6.7
1	B	159	LEU	6.5
1	A	288	ALA	5.8
1	B	164	HIS	5.8
1	A	482	SER	5.5
1	B	158	PHE	5.5
1	B	166	GLY	5.2
1	A	289	ASP	5.1
1	B	285	MET	5.1
1	A	396	ASP	5.1
1	A	159	LEU	4.8
1	B	262	SER	4.5
1	A	500	THR	4.5
1	A	157	THR	4.4
1	B	283	LYS	4.3
1	B	288	ALA	4.3
1	A	-2	GLY	4.2
1	A	204	ARG	4.2
1	B	181	ILE	4.1
1	A	158	PHE	4.0
1	A	29	GLY	3.9
1	B	163	ILE	3.8
1	A	291	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	204	ARG	3.8
1	A	154	THR	3.7
1	A	278	PRO	3.6
1	B	489	ALA	3.6
1	B	289	ASP	3.6
1	B	292	GLN	3.5
1	A	486	THR	3.5
1	B	345	TYR	3.4
1	A	489	ALA	3.4
1	B	396	ASP	3.4
1	B	500	THR	3.2
1	B	491	ALA	3.0
1	B	214	VAL	3.0
1	A	550	GLY	3.0
1	A	491	ALA	3.0
1	B	461	GLU	2.9
1	A	504	SER	2.9
1	A	522	LYS	2.9
1	A	290	ARG	2.9
1	A	498	HIS	2.9
1	A	287	PHE	2.7
1	A	165	ILE	2.6
1	B	256	ARG	2.6
1	A	496	ASN	2.6
1	B	475	ARG	2.6
1	B	370	GLN	2.6
1	A	125	VAL	2.5
1	B	342	ALA	2.5
1	A	471	GLU	2.5
1	B	293	HIS	2.5
1	B	477	ARG	2.5
1	A	285	MET	2.5
1	A	167	LEU	2.4
1	B	506	GLU	2.4
1	B	157	THR	2.3
1	A	397	ASP	2.3
1	B	160	ASP	2.3
1	A	494	GLU	2.3
1	A	395	SER	2.3
1	B	156	GLY	2.3
1	B	507	ALA	2.3
1	A	263	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	199	THR	2.3
1	A	30	GLN	2.3
1	B	30	GLN	2.3
1	B	249	GLU	2.3
1	B	287	PHE	2.3
1	B	329	GLN	2.3
1	A	540	GLU	2.3
1	A	502	PRO	2.3
1	A	525	THR	2.3
1	B	-1	SER	2.3
1	A	375	THR	2.2
1	A	180	SER	2.2
1	A	286	ARG	2.2
1	B	282	ASP	2.2
1	B	280	ILE	2.2
1	B	294	GLN	2.1
1	B	427	ARG	2.1
1	B	315	SER	2.1
1	B	502	PRO	2.1
1	A	249	GLU	2.1
1	B	180	SER	2.1
1	B	486	THR	2.1
1	A	516	PRO	2.1
1	A	36	THR	2.0
1	B	397	ASP	2.0
1	A	527	THR	2.0
1	B	421	GLY	2.0
1	A	505	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	552	5/5	0.92	0.19	79,79,79,80	0
2	SO4	B	1	5/5	0.93	0.12	77,78,78,78	0
2	SO4	A	551	5/5	0.94	0.12	71,72,72,72	0
2	SO4	B	551	5/5	0.94	0.23	85,85,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.