



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:34 AM UTC

PDB ID : 8I6Y / pdb_00008i6y
Title : Crystal structure of Arabidopsis thaliana LOX1
Authors : Liu, X.; Liu, L.
Deposited on : 2023-01-30
Resolution : 3.26 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
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

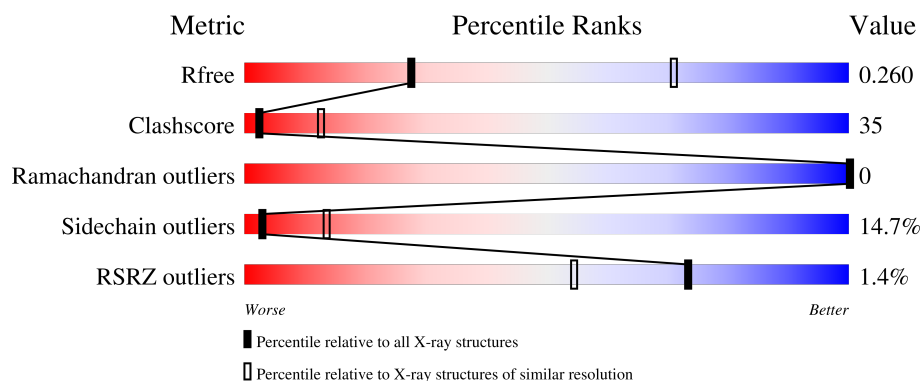
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	859	44% 43% 10% ..
1	B	859	2% 42% 45% 10% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13633 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 Linoleate 9S-lipoxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	0	0	0
			6810	4371	1132	1292	15			
1	B	844	Total	C	N	O	S	0	0	0
			6810	4371	1132	1292	15			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

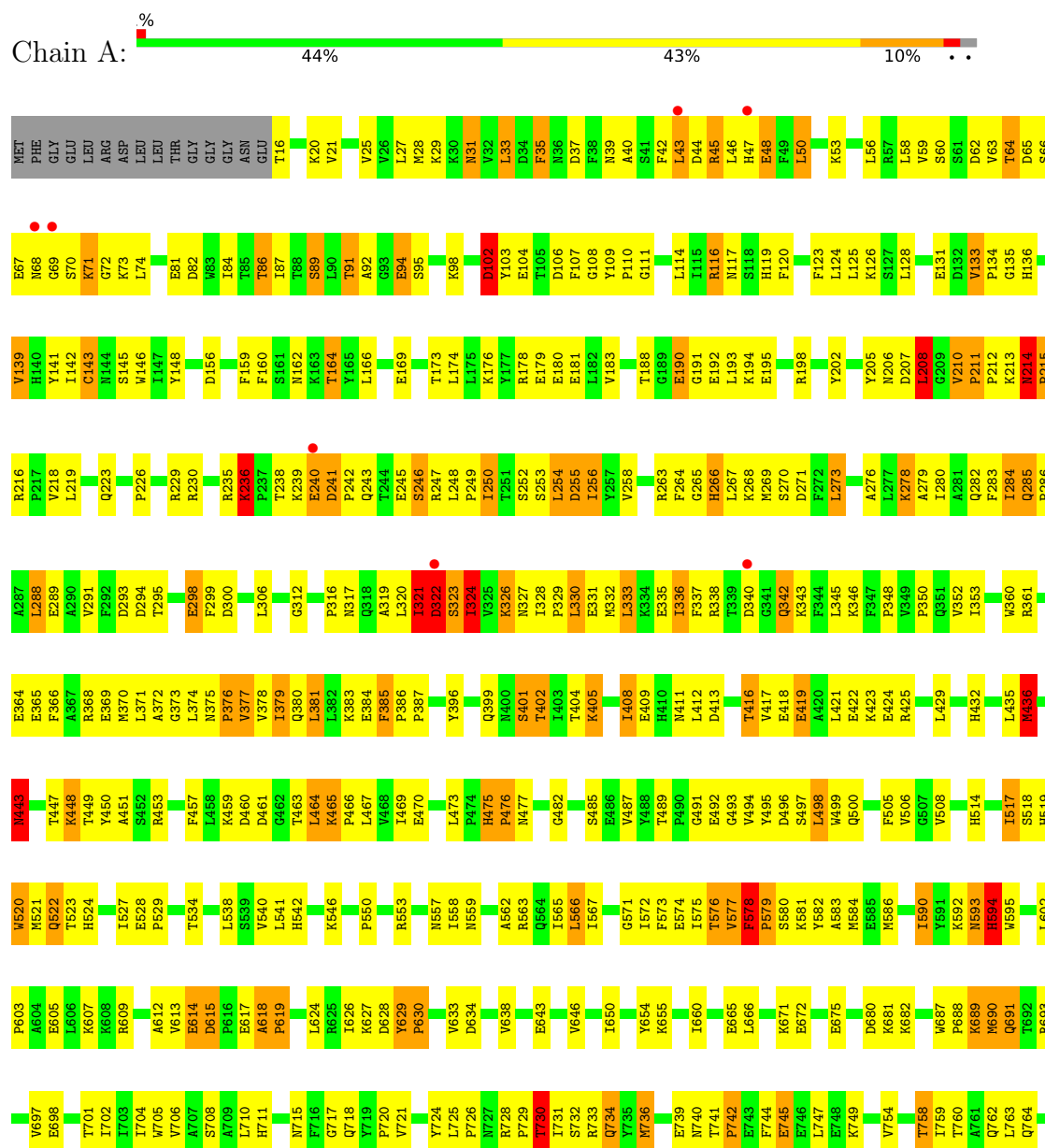
- Molecule 3 is water.

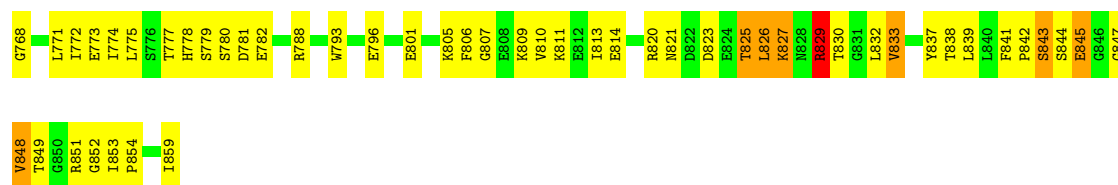
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	5	Total	O	0	0
			5	5		

3 Residue-property plots

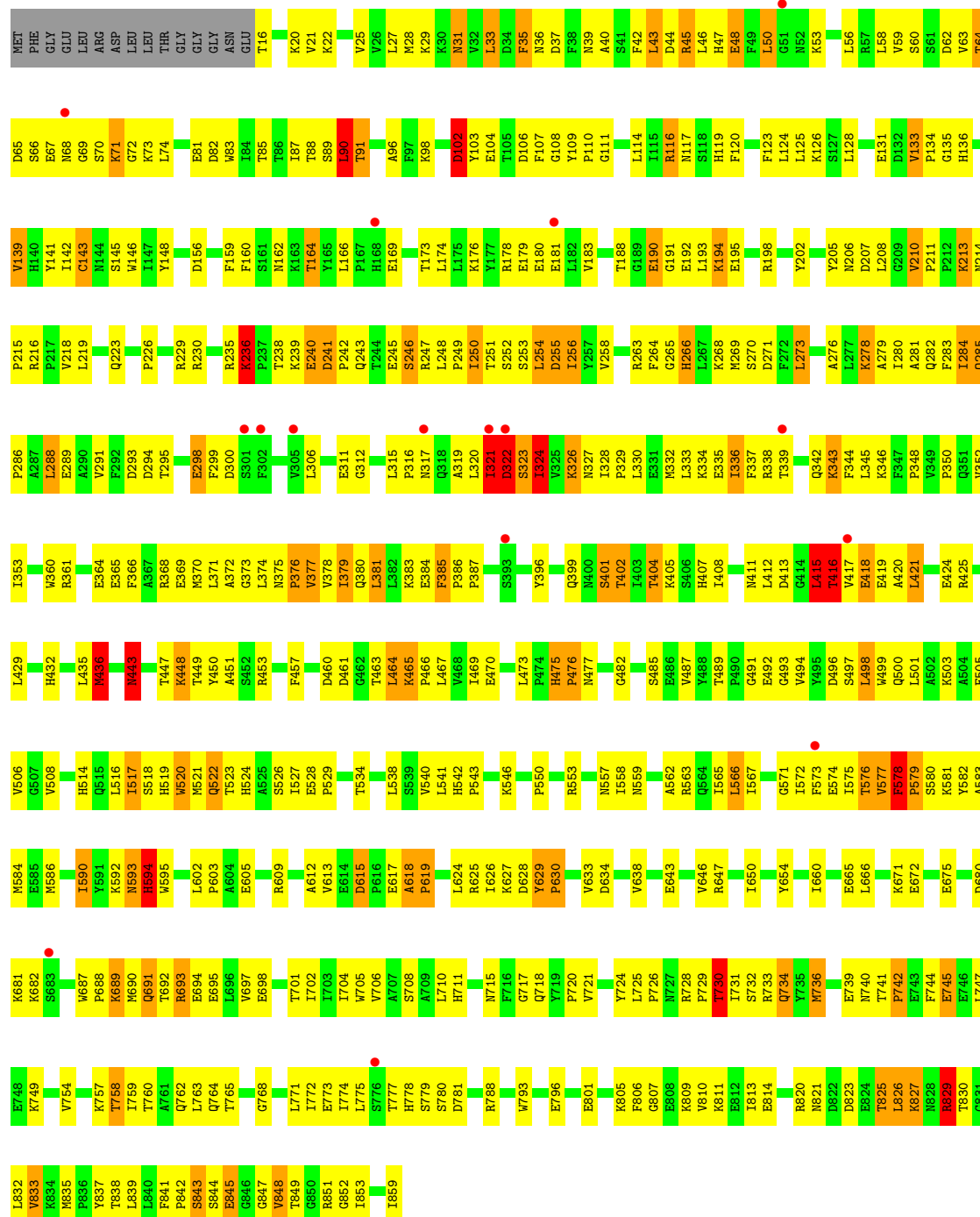
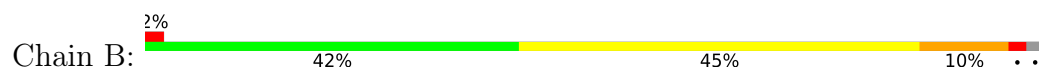
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Linoleate 9S-lipoxygenase 1





• Molecule 1: Linoleate 9S-lipoxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.37Å 119.35Å 135.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.68 – 3.26 67.68 – 3.26	Depositor EDS
% Data completeness (in resolution range)	95.8 (67.68-3.26) 95.7 (67.68-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.233 , 0.259 0.233 , 0.260	Depositor DCC
R_{free} test set	1380 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13633	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4147e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FE

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	1.04	32/6986 (0.5%)	1.15	83/9482 (0.9%)
1	B	1.04	30/6986 (0.4%)	1.16	89/9482 (0.9%)
All	All	1.04	62/13972 (0.4%)	1.16	172/18964 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	ASN	C-N	8.47	1.40	1.33
1	B	375	ASN	C-N	8.39	1.40	1.33
1	A	241	ASP	C-N	7.98	1.40	1.33
1	B	241	ASP	C-N	7.86	1.40	1.33
1	A	475	HIS	C-N	7.06	1.40	1.33
1	B	475	HIS	C-N	7.03	1.40	1.33
1	A	236	LYS	C-N	6.41	1.41	1.33
1	B	236	LYS	C-N	6.32	1.40	1.33
1	B	214	ASN	C-N	6.31	1.41	1.33
1	A	295	THR	C-N	6.29	1.40	1.33
1	B	295	THR	C-N	6.24	1.40	1.33
1	B	210	VAL	C-N	6.13	1.40	1.33
1	A	214	ASN	C-N	6.12	1.40	1.33
1	A	473	LEU	C-N	5.89	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	473	LEU	C-N	5.81	1.40	1.33
1	A	133	VAL	C-N	5.79	1.40	1.33
1	A	210	VAL	C-N	5.78	1.40	1.33
1	B	133	VAL	C-N	5.76	1.40	1.33
1	A	489	THR	C-N	5.63	1.41	1.33
1	B	489	THR	C-N	5.62	1.41	1.33
1	A	465	LYS	C-N	5.57	1.41	1.33
1	A	248	LEU	C-N	5.55	1.40	1.33
1	B	687	TRP	C-N	5.53	1.40	1.33
1	A	578	PHE	C-N	5.51	1.41	1.33
1	B	465	LYS	C-N	5.51	1.40	1.33
1	A	728	ARG	C-N	5.49	1.40	1.33
1	B	248	LEU	C-N	5.48	1.40	1.33
1	B	578	PHE	C-N	5.46	1.40	1.33
1	B	376	PRO	N-CD	5.45	1.55	1.47
1	B	728	ARG	C-N	5.42	1.40	1.33
1	A	376	PRO	N-CD	5.41	1.55	1.47
1	B	619	PRO	N-CD	5.40	1.55	1.47
1	A	615	ASP	C-N	5.37	1.40	1.34
1	B	742	PRO	N-CD	5.37	1.55	1.47
1	A	215	PRO	N-CD	5.36	1.55	1.47
1	A	619	PRO	N-CD	5.36	1.55	1.47
1	A	742	PRO	N-CD	5.35	1.55	1.47
1	A	687	TRP	C-N	5.34	1.40	1.33
1	B	853	ILE	C-N	5.34	1.40	1.33
1	A	853	ILE	C-N	5.27	1.40	1.33
1	B	629	TYR	C-N	5.26	1.41	1.34
1	A	629	TYR	C-N	5.19	1.41	1.34
1	A	436	MET	C-N	5.18	1.40	1.33
1	B	436	MET	C-N	5.15	1.40	1.33
1	A	211	PRO	N-CD	5.14	1.54	1.47
1	A	630	PRO	N-CD	5.14	1.54	1.47
1	B	211	PRO	C-N	5.13	1.41	1.34
1	B	630	PRO	N-CD	5.11	1.54	1.47
1	B	543	PRO	N-CD	5.10	1.54	1.47
1	A	211	PRO	C-N	5.09	1.41	1.34
1	B	134	PRO	N-CD	5.09	1.54	1.47
1	B	466	PRO	N-CD	5.08	1.54	1.47
1	B	729	PRO	N-CD	5.06	1.54	1.47
1	A	466	PRO	N-CD	5.05	1.54	1.47
1	A	729	PRO	N-CD	5.04	1.54	1.47
1	A	476	PRO	N-CD	5.04	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	PRO	N-CD	5.03	1.54	1.47
1	A	542	HIS	C-N	5.02	1.40	1.34
1	B	211	PRO	N-CD	5.01	1.54	1.47
1	B	476	PRO	N-CD	5.01	1.54	1.47
1	B	542	HIS	C-N	5.01	1.40	1.34
1	A	212	PRO	N-CD	5.01	1.54	1.47

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	ASP	N-CA-C	-10.76	98.19	111.11
1	B	322	ASP	N-CA-C	-10.73	98.23	111.11
1	A	321	ILE	CA-C-N	-9.39	107.86	120.54
1	A	321	ILE	C-N-CA	-9.39	107.86	120.54
1	B	321	ILE	CA-C-N	-9.36	107.91	120.54
1	B	321	ILE	C-N-CA	-9.36	107.91	120.54
1	A	323	SER	N-CA-C	8.95	120.64	111.07
1	B	323	SER	N-CA-C	8.95	120.64	111.07
1	A	336	ILE	N-CA-C	8.53	118.55	110.53
1	B	435	LEU	N-CA-C	8.49	120.62	111.36
1	A	435	LEU	N-CA-C	8.48	120.60	111.36
1	B	336	ILE	N-CA-C	8.47	118.49	110.53
1	A	520	TRP	N-CA-C	8.34	120.15	111.14
1	B	520	TRP	N-CA-C	8.34	120.14	111.14
1	B	416	THR	N-CA-C	-8.08	100.47	110.41
1	B	749	LYS	N-CA-C	7.89	119.66	111.14
1	A	749	LYS	N-CA-C	7.85	119.62	111.14
1	B	69	GLY	N-CA-C	-7.78	100.34	110.45
1	A	69	GLY	N-CA-C	-7.76	100.36	110.45
1	B	295	THR	CA-C-N	-7.37	113.09	120.31
1	B	295	THR	C-N-CA	-7.37	113.09	120.31
1	A	295	THR	CA-C-N	-7.34	113.12	120.31
1	A	295	THR	C-N-CA	-7.34	113.12	120.31
1	A	580	SER	CB-CA-C	-7.17	108.31	116.63
1	B	580	SER	CB-CA-C	-7.10	108.39	116.63
1	A	236	LYS	CA-C-N	-6.93	113.52	120.31
1	A	236	LYS	C-N-CA	-6.93	113.52	120.31
1	A	208	LEU	N-CA-C	6.89	118.79	111.28
1	B	236	LYS	CA-C-N	-6.89	113.56	120.31
1	B	236	LYS	C-N-CA	-6.89	113.56	120.31
1	B	594	HIS	N-CA-C	6.83	122.57	112.94
1	A	594	HIS	N-CA-C	6.80	122.53	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ASP	N-CA-C	6.78	118.75	111.36
1	B	62	ASP	N-CA-C	6.78	118.74	111.36
1	A	210	VAL	CA-C-N	-6.77	113.41	120.38
1	A	210	VAL	C-N-CA	-6.77	113.41	120.38
1	A	214	ASN	CA-C-N	-6.72	113.73	120.31
1	A	214	ASN	C-N-CA	-6.72	113.73	120.31
1	A	473	LEU	CA-C-N	-6.67	113.42	120.03
1	A	473	LEU	C-N-CA	-6.67	113.42	120.03
1	B	343	LYS	N-CA-C	-6.64	97.54	108.76
1	B	473	LEU	CA-C-N	-6.61	113.48	120.03
1	B	473	LEU	C-N-CA	-6.61	113.48	120.03
1	A	248	LEU	CA-C-N	-6.54	113.55	120.03
1	A	248	LEU	C-N-CA	-6.54	113.55	120.03
1	B	248	LEU	CA-C-N	-6.54	113.56	120.03
1	B	248	LEU	C-N-CA	-6.54	113.56	120.03
1	B	210	VAL	CA-C-N	-6.54	113.65	120.38
1	B	210	VAL	C-N-CA	-6.54	113.65	120.38
1	A	94	GLU	N-CA-C	-6.52	100.63	110.28
1	A	133	VAL	CA-C-N	-6.51	112.80	119.83
1	A	133	VAL	C-N-CA	-6.51	112.80	119.83
1	B	266	HIS	N-CA-C	-6.50	99.45	109.52
1	A	266	HIS	N-CA-C	-6.49	99.47	109.52
1	A	107	PHE	N-CA-C	6.49	118.43	111.36
1	B	107	PHE	N-CA-C	6.49	118.43	111.36
1	A	829	ARG	N-CA-C	6.47	118.33	111.28
1	A	728	ARG	CA-C-N	-6.47	113.10	119.76
1	A	728	ARG	C-N-CA	-6.47	113.10	119.76
1	B	133	VAL	CA-C-N	-6.47	112.84	119.83
1	B	133	VAL	C-N-CA	-6.47	112.84	119.83
1	B	829	ARG	N-CA-C	6.46	118.32	111.28
1	B	728	ARG	CA-C-N	-6.43	113.14	119.76
1	B	728	ARG	C-N-CA	-6.43	113.14	119.76
1	A	475	HIS	CA-C-N	-6.42	113.32	120.45
1	A	475	HIS	C-N-CA	-6.42	113.32	120.45
1	B	465	LYS	CA-C-N	-6.40	113.36	119.76
1	B	465	LYS	C-N-CA	-6.40	113.36	119.76
1	A	465	LYS	CA-C-N	-6.40	113.36	119.76
1	A	465	LYS	C-N-CA	-6.40	113.36	119.76
1	B	415	LEU	N-CA-C	-6.39	101.49	110.50
1	B	475	HIS	CA-C-N	-6.39	113.36	120.45
1	B	475	HIS	C-N-CA	-6.39	113.36	120.45
1	B	214	ASN	CA-C-N	-6.38	114.20	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ASN	C-N-CA	-6.38	114.20	120.52
1	A	730	THR	N-CA-C	6.20	117.84	111.14
1	B	489	THR	CA-C-N	-6.19	113.38	119.76
1	B	489	THR	C-N-CA	-6.19	113.38	119.76
1	B	208	LEU	N-CA-C	6.18	118.09	111.36
1	A	489	THR	CA-C-N	-6.17	113.40	119.76
1	A	489	THR	C-N-CA	-6.17	113.40	119.76
1	B	730	THR	N-CA-C	6.17	117.80	111.14
1	B	687	TRP	CA-C-N	-6.14	113.65	119.85
1	B	687	TRP	C-N-CA	-6.14	113.65	119.85
1	B	241	ASP	CA-C-N	-6.10	113.51	120.89
1	B	241	ASP	C-N-CA	-6.10	113.51	120.89
1	B	255	ASP	CA-C-N	6.10	128.67	120.50
1	B	255	ASP	C-N-CA	6.10	128.67	120.50
1	A	241	ASP	CA-C-N	-6.08	113.54	120.89
1	A	241	ASP	C-N-CA	-6.08	113.54	120.89
1	A	687	TRP	CA-C-N	-6.06	113.70	119.76
1	A	687	TRP	C-N-CA	-6.06	113.70	119.76
1	A	240	GLU	N-CA-C	6.03	117.93	111.36
1	B	240	GLU	N-CA-C	5.99	117.89	111.36
1	A	255	ASP	CA-C-N	5.94	128.61	120.35
1	A	255	ASP	C-N-CA	5.94	128.61	120.35
1	B	593	ASN	N-CA-C	5.88	117.77	111.36
1	B	375	ASN	CA-C-N	-5.88	114.18	121.00
1	B	375	ASN	C-N-CA	-5.88	114.18	121.00
1	A	375	ASN	CA-C-N	-5.88	114.18	121.00
1	A	375	ASN	C-N-CA	-5.88	114.18	121.00
1	A	593	ASN	N-CA-C	5.86	117.74	111.36
1	B	853	ILE	CA-C-N	-5.80	113.71	119.92
1	B	853	ILE	C-N-CA	-5.80	113.71	119.92
1	A	853	ILE	CA-C-N	-5.80	113.72	119.92
1	A	853	ILE	C-N-CA	-5.80	113.72	119.92
1	B	211	PRO	CA-C-N	-5.79	112.63	119.05
1	B	211	PRO	C-N-CA	-5.79	112.63	119.05
1	B	278	LYS	N-CA-C	-5.74	105.03	111.28
1	A	278	LYS	N-CA-C	-5.70	105.07	111.28
1	B	689	LYS	N-CA-C	5.69	117.56	111.36
1	B	90	LEU	N-CA-C	-5.66	105.12	111.28
1	B	377	VAL	N-CA-C	5.63	117.58	112.29
1	A	377	VAL	N-CA-C	5.55	117.51	112.29
1	B	741	THR	CA-C-N	-5.54	112.91	119.05
1	B	741	THR	C-N-CA	-5.54	112.91	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ILE	CB-CA-C	-5.53	104.78	112.02
1	B	336	ILE	CB-CA-C	-5.51	104.80	112.02
1	A	273	LEU	N-CA-C	-5.50	105.38	111.71
1	A	741	THR	CA-C-N	-5.50	112.94	119.05
1	A	741	THR	C-N-CA	-5.50	112.94	119.05
1	B	273	LEU	N-CA-C	-5.49	105.40	111.71
1	A	211	PRO	CA-C-N	-5.45	113.00	119.05
1	A	211	PRO	C-N-CA	-5.45	113.00	119.05
1	B	443	ASN	N-CA-C	5.44	119.18	112.54
1	B	693	ARG	N-CA-C	-5.43	105.36	111.28
1	A	443	ASN	N-CA-C	5.43	119.16	112.54
1	A	436	MET	CA-C-N	-5.38	113.37	119.28
1	A	436	MET	C-N-CA	-5.38	113.37	119.28
1	B	522	GLN	N-CA-C	5.36	117.20	111.36
1	A	522	GLN	N-CA-C	5.35	117.20	111.36
1	A	618	ALA	CA-C-N	-5.35	113.12	119.05
1	A	618	ALA	C-N-CA	-5.35	113.12	119.05
1	B	436	MET	CA-C-N	-5.34	113.40	119.28
1	B	436	MET	C-N-CA	-5.34	113.40	119.28
1	B	89	SER	N-CA-C	5.33	116.77	111.07
1	B	730	THR	CB-CA-C	-5.32	102.49	110.90
1	B	618	ALA	CA-C-N	-5.31	113.15	119.05
1	B	618	ALA	C-N-CA	-5.31	113.15	119.05
1	A	730	THR	CB-CA-C	-5.31	102.51	110.90
1	A	517	ILE	CB-CA-C	-5.29	104.99	111.92
1	B	517	ILE	CB-CA-C	-5.29	104.99	111.92
1	A	324	ILE	N-CA-C	5.28	115.50	110.53
1	B	324	ILE	N-CA-C	5.26	115.48	110.53
1	B	629	TYR	CA-C-N	-5.25	113.22	119.05
1	B	629	TYR	C-N-CA	-5.25	113.22	119.05
1	A	242	PRO	CA-N-CD	-5.24	104.66	112.00
1	B	242	PRO	CA-N-CD	-5.24	104.67	112.00
1	A	629	TYR	CA-C-N	-5.22	113.25	119.05
1	A	629	TYR	C-N-CA	-5.22	113.25	119.05
1	B	615	ASP	CA-C-N	-5.22	113.25	119.05
1	B	615	ASP	C-N-CA	-5.22	113.25	119.05
1	B	66	SER	N-CA-C	-5.12	105.70	111.28
1	A	66	SER	N-CA-C	-5.12	105.70	111.28
1	A	615	ASP	CA-C-N	-5.11	113.28	118.85
1	A	615	ASP	C-N-CA	-5.11	113.28	118.85
1	A	578	PHE	CA-C-N	-5.10	113.67	119.28
1	A	578	PHE	C-N-CA	-5.10	113.67	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	578	PHE	CA-C-N	-5.10	113.67	119.28
1	B	578	PHE	C-N-CA	-5.10	113.67	119.28
1	A	285	GLN	CA-C-N	-5.10	113.39	119.05
1	A	285	GLN	C-N-CA	-5.10	113.39	119.05
1	B	133	VAL	CB-CA-C	-5.09	106.01	111.00
1	A	579	PRO	CA-N-CD	-5.09	104.88	112.00
1	B	579	PRO	CA-N-CD	-5.08	104.88	112.00
1	B	285	GLN	CA-C-N	-5.08	113.41	119.05
1	B	285	GLN	C-N-CA	-5.08	113.41	119.05
1	A	102	ASP	N-CA-C	-5.04	100.30	108.41
1	B	102	ASP	N-CA-C	-5.03	100.31	108.41
1	A	688	PRO	CA-N-CD	-5.01	104.98	112.00
1	B	688	PRO	CA-N-CD	-5.01	104.98	112.00
1	A	87	ILE	N-CA-C	-5.00	105.52	110.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	ILE	Mainchain
1	B	321	ILE	Mainchain

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	6810	0	6696	461	2
1	B	6810	0	6696	483	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	0	2	0
3	B	5	0	0	4	0
All	All	13633	0	13392	944	2

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 35.

All (944) 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:381:LEU:CD2	1:A:383:LYS:HE3	1.57	1.33
1:B:381:LEU:CD2	1:B:383:LYS:HE3	1.57	1.33
1:B:311:GLU:O	1:B:343:LYS:CB	1.79	1.28
1:A:573:PHE:O	1:A:577:VAL:HG23	1.32	1.26
1:A:823:ASP:OD1	1:A:825:THR:HG22	1.12	1.25
1:B:823:ASP:OD1	1:B:825:THR:HG22	1.12	1.25
1:B:385:PHE:CE2	1:B:408:ILE:HD11	1.74	1.21
1:B:823:ASP:OD1	1:B:825:THR:CG2	1.90	1.19
1:A:823:ASP:OD1	1:A:825:THR:CG2	1.90	1.17
1:B:321:ILE:HA	1:B:324:ILE:CD1	1.74	1.17
1:A:321:ILE:HA	1:A:324:ILE:CD1	1.74	1.16
1:A:381:LEU:HD21	1:A:383:LYS:CE	1.77	1.14
1:B:385:PHE:HE2	1:B:408:ILE:HD11	0.99	1.14
1:B:415:LEU:HD22	1:B:419:GLU:HB3	1.19	1.14
1:A:782:GLU:OE2	1:A:854:PRO:HG3	1.45	1.14
1:A:782:GLU:OE2	1:A:854:PRO:CG	1.97	1.12
1:B:381:LEU:HD21	1:B:383:LYS:CE	1.77	1.12
1:B:254:LEU:HD22	1:B:255:ASP:H	1.15	1.11
1:A:254:LEU:HD22	1:A:255:ASP:H	1.16	1.11
1:A:321:ILE:O	1:A:322:ASP:C	1.88	1.11
1:B:385:PHE:HE2	1:B:408:ILE:CD1	1.61	1.11
1:A:192:GLU:OE2	1:A:236:LYS:HE2	1.51	1.10
1:A:498:LEU:HD12	1:A:736:MET:HE1	1.18	1.10
1:B:192:GLU:OE2	1:B:236:LYS:HE2	1.51	1.09
1:B:416:THR:HG23	1:B:419:GLU:H	1.08	1.07
1:B:263:ARG:HE	1:B:557:ASN:ND2	1.53	1.06
1:A:498:LEU:CD1	1:A:736:MET:HE1	1.85	1.06
1:B:321:ILE:O	1:B:322:ASP:C	1.88	1.05
1:B:65:ASP:HB2	1:B:73:LYS:HA	1.38	1.05
1:A:263:ARG:HE	1:A:557:ASN:ND2	1.53	1.05
1:A:565:ILE:HD12	1:A:566:LEU:HD12	1.38	1.05
1:B:321:ILE:HA	1:B:324:ILE:HD13	1.37	1.05
1:A:634:ASP:OD1	1:A:829:ARG:NH2	1.90	1.04
1:B:416:THR:N	1:B:419:GLU:OE1	1.90	1.04
1:B:634:ASP:OD1	1:B:829:ARG:NH2	1.90	1.03
1:A:250:ILE:HD12	1:A:250:ILE:H	1.20	1.03
1:A:65:ASP:HB2	1:A:73:LYS:HA	1.38	1.02
1:A:321:ILE:HA	1:A:324:ILE:HD13	1.37	1.02
1:B:71:LYS:O	1:B:173:THR:O	1.77	1.02
1:A:498:LEU:HD12	1:A:736:MET:CE	1.90	1.01
1:A:385:PHE:HE2	1:A:408:ILE:HD11	1.26	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:HD12	1:B:250:ILE:H	1.20	1.01
1:B:573:PHE:O	1:B:577:VAL:HG23	1.58	1.01
1:A:71:LYS:O	1:A:173:THR:O	1.77	1.01
1:A:754:VAL:O	1:A:758:THR:OG1	1.79	1.01
1:B:50:LEU:HD21	1:B:81:GLU:O	1.61	1.01
1:A:324:ILE:HD12	1:A:324:ILE:H	1.22	1.01
1:B:565:ILE:HD12	1:B:566:LEU:HD12	1.39	1.01
1:B:823:ASP:CG	1:B:825:THR:CG2	2.33	1.00
1:A:823:ASP:CG	1:A:825:THR:CG2	2.33	1.00
1:B:324:ILE:HD12	1:B:324:ILE:H	1.22	1.00
1:B:754:VAL:O	1:B:758:THR:OG1	1.79	1.00
1:B:415:LEU:HD22	1:B:419:GLU:CB	1.93	0.99
1:B:689:LYS:HA	1:B:689:LYS:HE2	1.40	0.99
1:A:148:TYR:OH	1:A:195:GLU:OE2	1.81	0.99
1:B:28:MET:HE1	1:B:33:LEU:HD11	1.46	0.98
1:B:45:ARG:HG2	1:B:45:ARG:HH11	1.29	0.97
1:B:416:THR:HG22	1:B:419:GLU:CD	1.89	0.97
1:A:425:ARG:NH2	1:A:460:ASP:OD1	1.97	0.97
1:B:425:ARG:NH2	1:B:460:ASP:OD1	1.97	0.97
1:B:143:CYS:HB3	1:B:159:PHE:CD1	2.00	0.97
1:A:28:MET:HE1	1:A:33:LEU:HD11	1.46	0.97
1:B:148:TYR:OH	1:B:195:GLU:OE2	1.81	0.96
1:B:443:ASN:HD21	1:B:449:THR:H	1.12	0.96
1:A:143:CYS:HB3	1:A:159:PHE:CD1	2.00	0.96
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.29	0.96
1:A:374:LEU:HB2	1:A:721:VAL:HG21	1.48	0.95
1:A:271:ASP:OD2	1:A:780:SER:OG	1.84	0.94
1:B:271:ASP:OD2	1:B:780:SER:OG	1.84	0.94
1:B:374:LEU:HB2	1:B:721:VAL:HG21	1.48	0.94
1:B:416:THR:HG23	1:B:419:GLU:N	1.82	0.94
1:B:565:ILE:CD1	1:B:566:LEU:HD12	1.98	0.94
1:A:565:ILE:CD1	1:A:566:LEU:HD12	1.98	0.93
1:B:381:LEU:HD21	1:B:383:LYS:HE3	0.94	0.93
1:A:68:ASN:ND2	1:A:74:LEU:HD11	1.84	0.93
1:B:289:GLU:O	1:B:293:ASP:HB2	1.69	0.92
1:B:263:ARG:HE	1:B:557:ASN:HD21	1.07	0.92
1:B:68:ASN:ND2	1:B:74:LEU:HD11	1.84	0.92
1:A:381:LEU:HD21	1:A:383:LYS:HE3	0.94	0.92
1:A:289:GLU:O	1:A:293:ASP:HB2	1.69	0.91
1:B:692:THR:OG1	1:B:695:GLU:HG3	1.70	0.91
1:A:250:ILE:O	1:A:282:GLN:NE2	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:O	1:B:282:GLN:NE2	2.04	0.91
1:A:263:ARG:NE	1:A:557:ASN:ND2	2.19	0.90
1:A:443:ASN:HD21	1:A:449:THR:H	1.12	0.90
1:A:263:ARG:HE	1:A:557:ASN:HD21	1.07	0.90
1:B:415:LEU:CD2	1:B:419:GLU:HB3	2.00	0.90
1:A:35:PHE:O	1:A:269:MET:HG2	1.71	0.90
1:A:68:ASN:ND2	1:A:74:LEU:CD1	2.35	0.90
1:A:475:HIS:HE1	1:A:477:ASN:HD22	1.15	0.90
1:B:35:PHE:O	1:B:269:MET:HG2	1.71	0.89
1:B:415:LEU:HD13	1:B:419:GLU:C	1.97	0.89
1:B:299:PHE:CZ	1:B:762:GLN:NE2	2.40	0.89
1:B:475:HIS:HE1	1:B:477:ASN:HD22	1.15	0.89
1:B:68:ASN:ND2	1:B:74:LEU:CD1	2.35	0.88
1:B:263:ARG:NE	1:B:557:ASN:ND2	2.19	0.88
1:B:321:ILE:HA	1:B:324:ILE:HD12	1.54	0.88
1:A:573:PHE:O	1:A:577:VAL:CG2	2.21	0.88
1:B:396:TYR:O	1:B:399:GLN:NE2	2.07	0.88
1:A:321:ILE:HA	1:A:324:ILE:HD12	1.54	0.88
1:A:299:PHE:CZ	1:A:762:GLN:NE2	2.40	0.87
1:A:298:GLU:OE1	1:A:733:ARG:NH2	2.07	0.87
1:A:396:TYR:O	1:A:399:GLN:NE2	2.07	0.87
1:A:263:ARG:HH21	1:A:557:ASN:ND2	1.72	0.87
1:B:116:ARG:HG2	1:B:116:ARG:HH11	1.39	0.87
1:A:266:HIS:ND1	1:A:781:ASP:OD2	2.08	0.87
1:B:263:ARG:HH21	1:B:557:ASN:ND2	1.72	0.87
1:B:298:GLU:OE1	1:B:733:ARG:NH2	2.07	0.86
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.39	0.86
1:B:68:ASN:HD22	1:B:74:LEU:CD1	1.89	0.86
1:B:385:PHE:HD1	1:B:386:PRO:N	1.74	0.86
1:A:68:ASN:HD22	1:A:74:LEU:CD1	1.89	0.85
1:B:266:HIS:ND1	1:B:781:ASP:OD2	2.08	0.85
1:A:208:LEU:HD13	1:A:567:ILE:O	1.77	0.85
1:A:385:PHE:HD1	1:A:386:PRO:N	1.74	0.85
1:A:86:THR:O	1:A:89:SER:OG	1.95	0.84
1:B:299:PHE:CE2	1:B:762:GLN:NE2	2.45	0.83
1:A:299:PHE:CE2	1:A:762:GLN:NE2	2.45	0.83
1:A:312:GLY:HA2	1:A:345:LEU:O	1.76	0.83
1:A:498:LEU:CD1	1:A:736:MET:CE	2.51	0.83
1:A:447:THR:O	1:A:448:LYS:HD2	1.79	0.83
1:B:249:PRO:HD2	1:B:252:SER:HB2	1.61	0.83
1:A:249:PRO:HD2	1:A:252:SER:HB2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PHE:CE2	1:A:408:ILE:HD11	2.13	0.83
1:B:415:LEU:HD13	1:B:420:ALA:N	1.93	0.83
1:B:447:THR:O	1:B:448:LYS:HD2	1.79	0.83
1:B:330:LEU:HD12	1:B:330:LEU:O	1.80	0.82
1:A:782:GLU:OE2	1:A:854:PRO:HG2	1.79	0.82
1:B:558:ILE:HD11	1:B:859:ILE:HD12	1.61	0.82
1:B:43:LEU:HD12	1:B:44:ASP:HA	1.61	0.82
1:A:254:LEU:HD22	1:A:255:ASP:N	1.95	0.81
1:B:823:ASP:OD2	1:B:825:THR:HG23	1.81	0.81
1:A:43:LEU:HD12	1:A:44:ASP:HA	1.61	0.81
1:A:690:MET:HE2	1:A:690:MET:HA	1.61	0.81
1:A:461:ASP:OD2	1:A:463:THR:HG23	1.81	0.81
1:A:823:ASP:OD2	1:A:825:THR:HG23	1.81	0.81
1:A:558:ILE:HD11	1:A:859:ILE:HD12	1.61	0.81
1:B:254:LEU:HD22	1:B:255:ASP:N	1.95	0.80
1:A:86:THR:N	1:A:89:SER:OG	2.15	0.80
1:B:236:LYS:O	1:B:246:SER:OG	1.99	0.80
1:A:236:LYS:O	1:A:246:SER:OG	1.99	0.80
1:A:443:ASN:HD21	1:A:449:THR:N	1.80	0.80
1:A:733:ARG:N	1:A:758:THR:O	2.15	0.79
1:B:461:ASP:OD2	1:B:463:THR:HG23	1.81	0.79
1:A:823:ASP:OD2	1:A:825:THR:CG2	2.30	0.79
1:B:263:ARG:NH2	1:B:557:ASN:ND2	2.31	0.78
1:B:443:ASN:HD21	1:B:449:THR:N	1.80	0.78
1:B:733:ARG:N	1:B:758:THR:O	2.15	0.78
1:B:82:ASP:O	1:B:98:LYS:N	2.15	0.78
1:B:823:ASP:OD2	1:B:825:THR:CG2	2.30	0.78
1:B:263:ARG:NE	1:B:557:ASN:HD21	1.80	0.78
1:A:263:ARG:NH2	1:A:557:ASN:ND2	2.31	0.78
1:A:660:ILE:HD12	1:A:693:ARG:HA	1.64	0.78
1:A:689:LYS:HA	1:A:689:LYS:CE	2.13	0.77
1:B:823:ASP:CG	1:B:825:THR:HG23	2.09	0.77
1:A:45:ARG:HG2	1:A:45:ARG:NH1	1.99	0.77
1:B:256:ILE:HD11	1:B:563:ARG:HH21	1.49	0.77
1:B:312:GLY:HA3	1:B:343:LYS:CB	2.13	0.77
1:A:312:GLY:CA	1:A:345:LEU:O	2.33	0.77
1:A:39:ASN:H	1:A:42:PHE:HD2	1.33	0.77
1:A:823:ASP:CG	1:A:825:THR:HG23	2.10	0.76
1:B:39:ASN:H	1:B:42:PHE:HD2	1.33	0.76
1:B:190:GLU:HG2	1:B:191:GLY:N	2.00	0.76
1:B:739:GLU:HA	1:B:744:PHE:CD2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLY:O	1:A:496:ASP:HB3	1.85	0.76
1:A:739:GLU:HA	1:A:744:PHE:CD2	2.20	0.76
1:A:28:MET:HE2	1:A:33:LEU:CD2	2.15	0.76
1:B:28:MET:HE2	1:B:33:LEU:CD2	2.16	0.76
1:B:449:THR:HG22	1:B:450:TYR:H	1.51	0.76
1:A:832:LEU:N	1:A:832:LEU:HD12	2.01	0.75
1:A:190:GLU:HG2	1:A:191:GLY:N	2.00	0.75
1:A:256:ILE:HD11	1:A:563:ARG:HH21	1.49	0.75
1:B:36:ASN:HB2	3:B:1003:HOH:O	1.84	0.75
1:A:449:THR:HG22	1:A:450:TYR:H	1.52	0.75
1:A:324:ILE:CD1	1:A:324:ILE:H	1.99	0.75
1:A:690:MET:HA	1:A:690:MET:CE	2.17	0.75
1:B:385:PHE:CE2	1:B:408:ILE:CD1	2.51	0.75
1:A:582:TYR:O	1:A:586:MET:HG3	1.86	0.75
1:B:374:LEU:HD11	1:B:718:GLN:HA	1.69	0.75
1:B:582:TYR:O	1:B:586:MET:HG3	1.86	0.75
1:B:321:ILE:CA	1:B:324:ILE:HD13	2.16	0.74
1:B:832:LEU:HD12	1:B:832:LEU:N	2.01	0.74
1:A:254:LEU:CD2	1:A:255:ASP:H	1.97	0.74
1:A:263:ARG:NE	1:A:557:ASN:HD21	1.80	0.74
1:A:321:ILE:CA	1:A:324:ILE:HD13	2.17	0.74
1:A:689:LYS:HA	1:A:689:LYS:HE2	1.67	0.74
1:B:109:TYR:HD2	1:B:136:HIS:CD2	2.05	0.74
1:B:324:ILE:CD1	1:B:324:ILE:H	1.99	0.74
1:B:385:PHE:CD1	1:B:386:PRO:N	2.56	0.74
1:A:84:ILE:C	1:A:84:ILE:HD12	2.13	0.74
1:B:28:MET:HE2	1:B:33:LEU:HD21	1.69	0.74
1:B:254:LEU:CD2	1:B:255:ASP:H	1.97	0.74
1:B:432:HIS:HA	1:B:451:ALA:HB1	1.70	0.74
1:A:517:ILE:HD11	1:A:590:ILE:HD12	1.69	0.73
1:A:381:LEU:HD23	1:A:383:LYS:HE3	1.69	0.73
1:B:424:GLU:OE1	1:B:625:ARG:NH1	2.21	0.73
1:A:374:LEU:HD11	1:A:718:GLN:HA	1.69	0.73
1:A:385:PHE:HE2	1:A:408:ILE:CD1	2.00	0.73
1:B:558:ILE:CD1	1:B:859:ILE:HD12	2.18	0.73
1:A:671:LYS:NZ	1:A:675:GLU:OE1	2.20	0.73
1:A:143:CYS:CB	1:A:159:PHE:CD1	2.72	0.73
1:A:28:MET:HE2	1:A:33:LEU:HD21	1.69	0.73
1:B:143:CYS:CB	1:B:159:PHE:CD1	2.72	0.73
1:A:558:ILE:CD1	1:A:859:ILE:HD12	2.18	0.72
1:B:517:ILE:HD11	1:B:590:ILE:HD12	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:HIS:O	1:B:50:LEU:HB2	1.89	0.72
1:A:385:PHE:CD1	1:A:386:PRO:N	2.56	0.72
1:A:47:HIS:O	1:A:50:LEU:HB2	1.89	0.72
1:B:416:THR:HG22	1:B:419:GLU:CG	2.20	0.72
1:A:109:TYR:HD2	1:A:136:HIS:CD2	2.05	0.72
1:B:16:THR:OG1	1:B:104:GLU:HG2	1.90	0.72
1:A:432:HIS:HA	1:A:451:ALA:HB1	1.70	0.72
1:B:814:GLU:OE2	1:B:843:SER:OG	2.08	0.72
1:B:116:ARG:HG2	1:B:116:ARG:NH1	2.04	0.71
1:A:16:THR:OG1	1:A:104:GLU:HG2	1.90	0.71
1:A:475:HIS:CE1	1:A:477:ASN:HD22	2.05	0.71
1:B:660:ILE:HD12	1:B:693:ARG:HA	1.71	0.71
1:B:321:ILE:O	1:B:322:ASP:O	2.08	0.71
1:A:208:LEU:CD1	1:A:567:ILE:O	2.38	0.71
1:A:342:GLN:HG3	1:A:342:GLN:O	1.91	0.71
1:A:416:THR:HG23	1:A:419:GLU:HB2	1.72	0.71
1:B:72:GLY:HA3	1:B:173:THR:HB	1.73	0.71
1:A:178:ARG:HH21	1:A:665:GLU:CD	1.99	0.70
1:A:814:GLU:OE2	1:A:843:SER:OG	2.08	0.70
1:B:178:ARG:HH21	1:B:665:GLU:CD	1.99	0.70
1:B:475:HIS:CE1	1:B:477:ASN:HD22	2.05	0.70
1:A:321:ILE:O	1:A:322:ASP:O	2.08	0.70
1:A:72:GLY:HA3	1:A:173:THR:HB	1.73	0.70
1:A:43:LEU:HD12	1:A:43:LEU:C	2.17	0.70
1:B:82:ASP:O	1:B:98:LYS:HB2	1.90	0.70
1:A:133:VAL:HG21	1:A:139:VAL:CG1	2.22	0.70
1:B:45:ARG:HG2	1:B:45:ARG:NH1	1.99	0.70
1:B:133:VAL:HG21	1:B:139:VAL:CG1	2.22	0.70
1:B:43:LEU:HD12	1:B:43:LEU:C	2.17	0.69
1:B:814:GLU:CD	1:B:843:SER:OG	2.35	0.69
1:B:20:LYS:HD3	1:B:102:ASP:OD1	1.93	0.69
1:B:321:ILE:HG22	1:B:324:ILE:HD13	1.74	0.69
1:A:814:GLU:CD	1:A:843:SER:OG	2.35	0.69
1:B:572:ILE:O	1:B:576:THR:OG1	2.10	0.69
1:A:116:ARG:HG2	1:A:116:ARG:NH1	2.04	0.69
1:B:324:ILE:HD12	1:B:324:ILE:N	2.04	0.69
1:B:322:ASP:O	1:B:326:LYS:HB2	1.91	0.69
1:B:827:LYS:N	1:B:827:LYS:HD3	2.08	0.69
1:A:321:ILE:HG22	1:A:324:ILE:HD13	1.74	0.69
1:A:322:ASP:O	1:A:326:LYS:HB2	1.91	0.69
1:B:517:ILE:O	1:B:522:GLN:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:MET:HE1	1:A:33:LEU:CD1	2.23	0.68
1:B:216:ARG:NH2	1:B:574:GLU:OE2	2.20	0.68
1:A:517:ILE:O	1:A:522:GLN:HG3	1.93	0.68
1:A:572:ILE:O	1:A:576:THR:OG1	2.11	0.68
1:B:273:LEU:HD22	1:B:777:THR:OG1	1.93	0.68
1:A:143:CYS:HB3	1:A:159:PHE:HD1	1.56	0.68
1:A:250:ILE:H	1:A:250:ILE:CD1	1.96	0.68
1:A:263:ARG:CZ	1:A:557:ASN:ND2	2.57	0.68
1:A:827:LYS:HD3	1:A:827:LYS:N	2.08	0.68
1:B:43:LEU:HD12	1:B:44:ASP:CA	2.24	0.68
1:B:660:ILE:CD1	1:B:693:ARG:HA	2.24	0.68
1:A:20:LYS:HD3	1:A:102:ASP:OD1	1.93	0.68
1:B:387:PRO:O	1:B:401:SER:OG	2.12	0.68
1:B:250:ILE:H	1:B:250:ILE:CD1	1.96	0.68
1:A:273:LEU:HD22	1:A:777:THR:OG1	1.93	0.68
1:B:263:ARG:CZ	1:B:557:ASN:ND2	2.57	0.68
1:A:50:LEU:HD21	1:A:81:GLU:O	1.93	0.67
1:B:671:LYS:NZ	1:B:675:GLU:OE1	2.20	0.67
1:B:381:LEU:HD23	1:B:383:LYS:HE3	1.69	0.67
1:A:43:LEU:HD12	1:A:44:ASP:CA	2.24	0.67
1:B:498:LEU:CD1	1:B:747:LEU:HD21	2.24	0.67
1:B:50:LEU:CD2	1:B:81:GLU:O	2.40	0.67
1:A:387:PRO:O	1:A:401:SER:OG	2.12	0.66
1:B:385:PHE:CD1	1:B:386:PRO:CA	2.78	0.66
1:B:64:THR:HA	1:B:72:GLY:HA2	1.78	0.66
1:B:566:LEU:O	1:B:573:PHE:HB2	1.94	0.66
1:A:660:ILE:CD1	1:A:693:ARG:HA	2.25	0.66
1:B:278:LYS:O	1:B:282:GLN:HG3	1.96	0.66
1:B:28:MET:HE1	1:B:33:LEU:CD1	2.23	0.66
1:A:278:LYS:O	1:A:282:GLN:HG3	1.96	0.66
1:A:306:LEU:HD21	1:A:353:ILE:HD11	1.78	0.66
1:B:415:LEU:HD22	1:B:419:GLU:CG	2.25	0.66
1:A:385:PHE:CD1	1:A:386:PRO:CA	2.78	0.65
1:B:306:LEU:HD21	1:B:353:ILE:HD11	1.78	0.65
1:B:519:HIS:O	1:B:523:THR:OG1	2.14	0.65
1:A:273:LEU:CD2	1:A:777:THR:OG1	2.45	0.65
1:A:64:THR:HA	1:A:72:GLY:HA2	1.77	0.65
1:A:71:LYS:NZ	1:A:180:GLU:OE1	2.30	0.64
1:A:519:HIS:O	1:A:523:THR:OG1	2.14	0.64
1:A:338:ARG:HB2	1:A:346:LYS:HB3	1.80	0.64
1:B:71:LYS:NZ	1:B:180:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LEU:CD2	1:B:777:THR:OG1	2.45	0.64
1:A:374:LEU:HD13	1:A:721:VAL:HG22	1.79	0.64
1:A:447:THR:C	1:A:448:LYS:HD2	2.22	0.64
1:A:704:ILE:O	1:A:708:SER:OG	2.12	0.64
1:B:143:CYS:HB3	1:B:159:PHE:HD1	1.56	0.64
1:B:28:MET:CE	1:B:33:LEU:HD11	2.26	0.64
1:A:336:ILE:HG12	1:A:774:ILE:HD11	1.80	0.64
1:B:385:PHE:CD1	1:B:386:PRO:HA	2.33	0.64
1:B:448:LYS:O	1:B:732:SER:OG	2.16	0.64
1:A:814:GLU:HG3	1:A:842:PRO:HD2	1.80	0.64
1:B:447:THR:C	1:B:448:LYS:HD2	2.22	0.64
1:B:374:LEU:HD13	1:B:721:VAL:HG22	1.79	0.63
1:A:385:PHE:CD1	1:A:386:PRO:HA	2.32	0.63
1:A:841:PHE:O	1:A:852:GLY:HA2	1.98	0.63
1:A:216:ARG:NH1	1:A:581:LYS:HG3	2.14	0.63
1:A:312:GLY:CA	1:A:343:LYS:CB	2.76	0.63
1:B:250:ILE:HD12	1:B:250:ILE:N	2.04	0.63
1:A:206:ASN:OD1	1:A:206:ASN:N	2.32	0.63
1:A:448:LYS:O	1:A:732:SER:OG	2.16	0.63
1:A:35:PHE:HZ	1:A:332:MET:HE1	1.63	0.63
1:A:103:TYR:OH	1:A:108:GLY:O	2.17	0.63
1:A:39:ASN:ND2	1:A:40:ALA:H	1.96	0.63
1:A:571:GLY:O	1:A:575:ILE:HG12	1.99	0.63
1:B:35:PHE:HZ	1:B:332:MET:HE1	1.63	0.63
1:B:336:ILE:HG12	1:B:774:ILE:HD11	1.80	0.63
1:A:324:ILE:HD12	1:A:324:ILE:N	2.04	0.62
1:A:235:ARG:HB2	1:A:245:GLU:OE2	1.99	0.62
1:A:660:ILE:HD11	1:A:693:ARG:HG2	1.81	0.62
1:B:39:ASN:ND2	1:B:40:ALA:H	1.96	0.62
1:B:841:PHE:O	1:B:852:GLY:HA2	1.98	0.62
1:B:814:GLU:HG3	1:B:842:PRO:HD2	1.80	0.62
1:A:28:MET:CE	1:A:33:LEU:HD11	2.26	0.62
1:B:206:ASN:OD1	1:B:206:ASN:N	2.32	0.62
1:A:43:LEU:HD12	1:A:44:ASP:N	2.15	0.62
1:A:241:ASP:OD1	1:A:243:GLN:HG2	2.00	0.62
1:B:43:LEU:HD12	1:B:44:ASP:N	2.15	0.62
1:B:416:THR:N	1:B:419:GLU:HB2	2.14	0.62
1:B:235:ARG:HB2	1:B:245:GLU:OE2	1.99	0.61
1:A:240:GLU:CD	1:A:240:GLU:H	2.09	0.61
1:A:250:ILE:HD12	1:A:250:ILE:N	2.04	0.61
1:A:405:LYS:O	1:A:409:GLU:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:TYR:OH	1:B:108:GLY:O	2.17	0.61
1:B:241:ASP:OD1	1:B:243:GLN:HG2	2.00	0.61
1:B:321:ILE:CA	1:B:324:ILE:CD1	2.66	0.61
1:B:689:LYS:HE2	1:B:689:LYS:CA	2.21	0.61
1:A:693:ARG:O	1:A:697:VAL:HG23	2.01	0.61
1:B:162:ASN:O	1:B:546:LYS:NZ	2.35	0.60
1:A:216:ARG:NH1	1:A:581:LYS:HE3	2.16	0.60
1:A:162:ASN:O	1:A:546:LYS:NZ	2.35	0.60
1:B:126:LYS:O	1:B:143:CYS:O	2.19	0.60
1:B:571:GLY:O	1:B:575:ILE:HG12	2.01	0.60
1:A:402:THR:HG21	1:A:485:SER:HB2	1.84	0.60
1:A:126:LYS:O	1:A:143:CYS:O	2.19	0.60
1:B:374:LEU:HB2	1:B:721:VAL:CG2	2.28	0.60
1:A:214:ASN:OD1	1:A:214:ASN:N	2.35	0.60
1:B:823:ASP:CG	1:B:825:THR:HG22	2.00	0.60
1:A:374:LEU:HB2	1:A:721:VAL:CG2	2.28	0.60
1:B:558:ILE:HD13	1:B:859:ILE:HA	1.84	0.60
1:A:229:ARG:NH1	1:A:680:ASP:OD2	2.26	0.59
1:B:240:GLU:H	1:B:240:GLU:CD	2.09	0.59
1:B:315:LEU:HD21	1:B:345:LEU:HD11	1.84	0.59
1:B:593:ASN:CB	1:B:594:HIS:CD2	2.85	0.59
1:A:92:ALA:HA	1:A:267:LEU:HD21	1.84	0.59
1:A:593:ASN:CB	1:A:594:HIS:CD2	2.85	0.59
1:A:84:ILE:HD12	1:A:84:ILE:O	2.01	0.59
1:A:312:GLY:HA3	1:A:343:LYS:CB	2.33	0.59
1:A:832:LEU:HD12	1:A:832:LEU:H	1.68	0.59
1:B:65:ASP:CB	1:B:73:LYS:HA	2.25	0.59
1:A:498:LEU:CG	1:A:736:MET:HE1	2.33	0.59
1:B:704:ILE:O	1:B:708:SER:OG	2.12	0.59
1:A:366:PHE:HZ	1:A:506:VAL:HG21	1.68	0.59
1:B:725:LEU:HB3	1:B:726:PRO:HD3	1.85	0.59
1:B:366:PHE:HZ	1:B:506:VAL:HG21	1.68	0.59
1:A:494:VAL:O	1:A:497:SER:HB2	2.03	0.58
1:B:402:THR:HG21	1:B:485:SER:HB2	1.84	0.58
1:B:312:GLY:CA	1:B:343:LYS:CB	2.80	0.58
1:B:581:LYS:CE	3:B:1004:HOH:O	2.51	0.58
1:B:832:LEU:HD12	1:B:832:LEU:H	1.68	0.58
1:A:245:GLU:HG3	3:A:1005:HOH:O	2.03	0.58
1:A:634:ASP:CG	1:A:829:ARG:NH2	2.61	0.58
1:B:133:VAL:HG21	1:B:139:VAL:HG13	1.85	0.58
1:B:764:GLN:N	1:B:764:GLN:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ILE:HD13	1:A:859:ILE:HA	1.84	0.58
1:B:166:LEU:HB2	1:B:169:GLU:HG2	1.85	0.58
1:A:133:VAL:HG21	1:A:139:VAL:HG13	1.85	0.58
1:B:229:ARG:NH1	1:B:680:ASP:OD2	2.26	0.58
1:B:654:TYR:CD1	1:B:660:ILE:HG12	2.39	0.58
1:A:206:ASN:HB3	1:A:218:VAL:HG13	1.85	0.58
1:A:523:THR:OG1	1:A:524:HIS:N	2.35	0.58
1:A:763:LEU:HB3	1:A:764:GLN:OE1	2.04	0.58
1:A:848:VAL:HG22	1:A:848:VAL:O	2.03	0.58
1:B:475:HIS:HE1	1:B:477:ASN:ND2	1.96	0.58
1:B:593:ASN:CB	1:B:594:HIS:HD2	2.17	0.58
1:A:28:MET:CE	1:A:33:LEU:HD21	2.34	0.58
1:A:654:TYR:CD1	1:A:660:ILE:HG12	2.39	0.58
1:B:321:ILE:HG21	1:B:344:PHE:CD2	2.39	0.58
1:A:417:VAL:HG23	1:A:418:GLU:N	2.18	0.58
1:B:33:LEU:O	1:B:265:GLY:HA3	2.04	0.58
1:A:65:ASP:CB	1:A:73:LYS:HA	2.25	0.57
1:A:216:ARG:NH2	1:A:574:GLU:OE2	2.36	0.57
1:B:206:ASN:HB3	1:B:218:VAL:HG13	1.85	0.57
1:B:848:VAL:HG22	1:B:848:VAL:O	2.03	0.57
1:A:166:LEU:HB2	1:A:169:GLU:HG2	1.85	0.57
1:B:634:ASP:CG	1:B:829:ARG:NH2	2.61	0.57
1:B:763:LEU:HB3	1:B:764:GLN:OE1	2.04	0.57
1:B:210:VAL:HB	1:B:213:LYS:O	2.04	0.57
1:B:379:ILE:O	1:B:609:ARG:HD2	2.05	0.57
1:A:33:LEU:O	1:A:265:GLY:HA3	2.04	0.57
1:A:725:LEU:HB3	1:A:726:PRO:HD3	1.85	0.57
1:B:594:HIS:CD2	1:B:594:HIS:N	2.73	0.57
1:A:379:ILE:O	1:A:609:ARG:HD2	2.04	0.57
1:A:764:GLN:OE1	1:A:764:GLN:N	2.37	0.57
1:B:424:GLU:CD	1:B:625:ARG:HH11	2.13	0.57
1:A:469:ILE:HG13	1:A:499:TRP:CZ3	2.40	0.57
1:B:28:MET:CE	1:B:33:LEU:HD21	2.34	0.57
1:B:288:LEU:HB3	1:B:763:LEU:CD1	2.35	0.57
1:A:288:LEU:HB3	1:A:763:LEU:CD1	2.35	0.57
1:A:594:HIS:CD2	1:A:594:HIS:N	2.73	0.57
1:A:814:GLU:HG2	1:A:841:PHE:CZ	2.40	0.57
1:B:469:ILE:HG13	1:B:499:TRP:CZ3	2.40	0.57
1:A:706:VAL:HG13	1:A:710:LEU:HD23	1.87	0.56
1:B:109:TYR:CD2	1:B:136:HIS:CD2	2.92	0.56
1:B:117:ASN:ND2	1:B:123:PHE:CE1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:VAL:HG13	1:B:710:LEU:HD23	1.87	0.56
1:A:321:ILE:CA	1:A:324:ILE:CD1	2.66	0.56
1:A:593:ASN:CB	1:A:594:HIS:HD2	2.17	0.56
1:B:181:GLU:OE2	1:B:198:ARG:NH2	2.28	0.56
1:B:814:GLU:HG2	1:B:841:PHE:CZ	2.40	0.56
1:A:283:PHE:CE2	1:A:327:ASN:HB3	2.40	0.56
1:A:312:GLY:C	1:A:343:LYS:CB	2.79	0.56
1:A:607:LYS:HE3	1:A:614:GLU:OE1	2.05	0.56
1:A:717:GLY:C	1:A:720:PRO:HD2	2.31	0.56
1:B:453:ARG:NH1	1:B:470:GLU:OE2	2.37	0.56
1:A:230:ARG:HD3	1:A:563:ARG:CZ	2.36	0.56
1:B:523:THR:OG1	1:B:524:HIS:N	2.35	0.56
1:B:283:PHE:CE2	1:B:327:ASN:HB3	2.40	0.56
1:A:31:ASN:OD1	1:A:31:ASN:N	2.33	0.56
1:B:207:ASP:O	1:B:247:ARG:HD2	2.06	0.56
1:B:230:ARG:HD3	1:B:563:ARG:CZ	2.36	0.56
1:B:572:ILE:HG21	1:B:771:LEU:HD13	1.88	0.56
1:A:117:ASN:ND2	1:A:123:PHE:CE1	2.73	0.56
1:B:114:LEU:HD22	1:B:156:ASP:HB2	1.88	0.56
1:B:263:ARG:NH2	1:B:557:ASN:HD22	2.03	0.56
1:B:505:PHE:HZ	1:B:734:GLN:O	1.89	0.56
1:A:50:LEU:CD2	1:A:81:GLU:O	2.54	0.56
1:A:282:GLN:O	1:A:286:PRO:HG2	2.05	0.56
1:B:282:GLN:O	1:B:286:PRO:HG2	2.05	0.56
1:A:35:PHE:O	1:A:269:MET:CG	2.51	0.55
1:B:581:LYS:HE3	3:B:1004:HOH:O	2.06	0.55
1:B:717:GLY:C	1:B:720:PRO:HD2	2.31	0.55
1:B:742:PRO:O	1:B:745:GLU:HB2	2.06	0.55
1:A:744:PHE:HD1	1:A:744:PHE:O	1.90	0.55
1:B:385:PHE:HE2	1:B:408:ILE:HD13	1.65	0.55
1:A:146:TRP:HE1	1:A:264:PHE:HD2	1.54	0.55
1:A:385:PHE:CD1	1:A:385:PHE:C	2.85	0.55
1:A:742:PRO:O	1:A:745:GLU:HB2	2.06	0.55
1:A:374:LEU:CD1	1:A:718:GLN:HA	2.37	0.55
1:B:415:LEU:CD1	1:B:420:ALA:HA	2.36	0.55
1:B:146:TRP:HE1	1:B:264:PHE:HD2	1.53	0.55
1:B:385:PHE:CD1	1:B:385:PHE:C	2.85	0.55
1:B:689:LYS:HA	1:B:689:LYS:CE	2.25	0.55
1:A:505:PHE:HZ	1:A:734:GLN:O	1.89	0.55
1:B:330:LEU:HD12	1:B:330:LEU:C	2.32	0.55
1:B:241:ASP:OD1	1:B:243:GLN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:PHE:HD1	1:B:744:PHE:O	1.90	0.55
1:A:114:LEU:HD22	1:A:156:ASP:HB2	1.88	0.55
1:A:578:PHE:C	1:A:578:PHE:CD2	2.85	0.55
1:B:202:TYR:HE2	1:B:672:GLU:OE1	1.90	0.55
1:A:109:TYR:HD2	1:A:136:HIS:HD2	1.51	0.54
1:A:572:ILE:HG21	1:A:771:LEU:HD13	1.87	0.54
1:A:202:TYR:HE2	1:A:672:GLU:OE1	1.90	0.54
1:A:207:ASP:O	1:A:247:ARG:HD2	2.06	0.54
1:A:494:VAL:O	1:A:497:SER:N	2.39	0.54
1:B:366:PHE:CZ	1:B:506:VAL:HG21	2.43	0.54
1:B:693:ARG:O	1:B:697:VAL:HG23	2.07	0.54
1:B:344:PHE:CD1	1:B:344:PHE:C	2.85	0.54
1:A:39:ASN:HD22	1:A:40:ALA:H	1.56	0.54
1:B:31:ASN:N	1:B:31:ASN:OD1	2.33	0.54
1:B:416:THR:H	1:B:419:GLU:HB2	1.73	0.54
1:A:453:ARG:NH1	1:A:470:GLU:OE2	2.37	0.54
1:A:181:GLU:OE2	1:A:198:ARG:NH2	2.28	0.54
1:A:443:ASN:O	1:A:448:LYS:HE3	2.08	0.54
1:A:739:GLU:HA	1:A:744:PHE:HD2	1.71	0.54
1:B:321:ILE:CG2	1:B:324:ILE:HD13	2.38	0.54
1:B:578:PHE:C	1:B:578:PHE:CD2	2.85	0.54
1:A:520:TRP:CZ2	1:A:567:ILE:HD13	2.43	0.54
1:A:366:PHE:CZ	1:A:506:VAL:HG21	2.43	0.53
1:A:607:LYS:CE	1:A:614:GLU:OE2	2.56	0.53
1:A:216:ARG:CZ	1:A:581:LYS:HG3	2.39	0.53
1:A:689:LYS:HA	1:A:689:LYS:HE3	1.89	0.53
1:B:21:VAL:HG13	1:B:131:GLU:O	2.09	0.53
1:B:415:LEU:HD13	1:B:419:GLU:HB3	1.90	0.53
1:A:91:THR:O	1:A:92:ALA:HB3	2.08	0.53
1:A:821:ASN:OD1	1:A:829:ARG:HG2	2.08	0.53
1:B:411:ASN:C	1:B:412:LEU:HD23	2.33	0.53
1:B:520:TRP:CZ2	1:B:567:ILE:HD13	2.43	0.53
1:B:821:ASN:OD1	1:B:829:ARG:HG2	2.08	0.53
1:A:263:ARG:CZ	1:A:557:ASN:HD22	2.22	0.53
1:B:160:PHE:HB3	1:B:541:LEU:HD21	1.91	0.53
1:A:494:VAL:HG13	1:A:495:TYR:N	2.23	0.53
1:A:607:LYS:HE3	1:A:614:GLU:OE2	2.08	0.53
1:B:190:GLU:HG2	1:B:191:GLY:H	1.74	0.53
1:B:374:LEU:CD1	1:B:718:GLN:HA	2.37	0.53
1:A:21:VAL:HG13	1:A:131:GLU:O	2.09	0.53
1:A:321:ILE:CG2	1:A:324:ILE:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:HD22	1:B:40:ALA:H	1.56	0.53
1:B:90:LEU:O	1:B:90:LEU:HD12	2.09	0.53
1:B:416:THR:HG22	1:B:419:GLU:OE1	2.09	0.53
1:A:160:PHE:HB3	1:A:541:LEU:HD21	1.91	0.53
1:B:491:GLY:O	1:B:496:ASP:HB2	2.09	0.53
1:B:595:TRP:O	1:B:681:LYS:HE2	2.09	0.53
1:B:807:GLY:O	1:B:811:LYS:HG3	2.09	0.53
1:A:283:PHE:C	1:A:286:PRO:HD2	2.34	0.52
1:B:385:PHE:HD1	1:B:385:PHE:C	2.17	0.52
1:B:417:VAL:HG23	1:B:418:GLU:OE2	2.08	0.52
1:A:111:GLY:HA3	1:A:174:LEU:HD11	1.91	0.52
1:A:263:ARG:NH2	1:A:557:ASN:HD22	2.03	0.52
1:B:443:ASN:O	1:B:448:LYS:HE3	2.08	0.52
1:B:207:ASP:O	1:B:247:ARG:CD	2.58	0.52
1:B:263:ARG:CZ	1:B:557:ASN:HD22	2.22	0.52
1:A:28:MET:CE	1:A:33:LEU:CD1	2.86	0.52
1:A:218:VAL:O	1:A:219:LEU:HD23	2.09	0.52
1:A:517:ILE:HG23	1:A:521:MET:HE3	1.91	0.52
1:A:595:TRP:O	1:A:681:LYS:HE2	2.09	0.52
1:A:634:ASP:OD1	1:A:820:ARG:NH2	2.43	0.52
1:B:111:GLY:HA3	1:B:174:LEU:HD11	1.91	0.52
1:A:109:TYR:CD2	1:A:136:HIS:CD2	2.92	0.52
1:A:593:ASN:HB2	1:A:594:HIS:HD2	1.75	0.52
1:A:607:LYS:HE3	1:A:614:GLU:CD	2.35	0.52
1:B:109:TYR:HD2	1:B:136:HIS:HD2	1.51	0.52
1:A:71:LYS:O	1:A:173:THR:C	2.52	0.52
1:B:534:THR:HG23	1:B:538:LEU:HD12	1.92	0.52
1:A:241:ASP:OD1	1:A:243:GLN:N	2.40	0.52
1:B:218:VAL:O	1:B:219:LEU:HD23	2.09	0.52
1:A:190:GLU:HG2	1:A:191:GLY:H	1.74	0.52
1:A:317:ASN:HD22	1:A:319:ALA:HB3	1.75	0.52
1:B:35:PHE:O	1:B:269:MET:CG	2.51	0.52
1:B:68:ASN:HD21	1:B:74:LEU:HD11	1.73	0.52
1:A:207:ASP:O	1:A:247:ARG:CD	2.58	0.52
1:A:807:GLY:O	1:A:811:LYS:HG3	2.09	0.52
1:B:517:ILE:HG23	1:B:521:MET:HE3	1.91	0.52
1:B:365:GLU:CD	1:B:368:ARG:HE	2.18	0.51
1:B:416:THR:H	1:B:419:GLU:CD	2.09	0.51
1:B:565:ILE:HD11	1:B:566:LEU:HD12	1.89	0.51
1:A:254:LEU:HD13	1:A:255:ASP:O	2.10	0.51
1:B:317:ASN:HD22	1:B:319:ALA:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:THR:O	1:A:827:LYS:NZ	2.29	0.51
1:B:28:MET:CE	1:B:33:LEU:CD1	2.87	0.51
1:B:634:ASP:OD1	1:B:820:ARG:NH2	2.43	0.51
1:A:33:LEU:HB3	1:A:265:GLY:HA3	1.92	0.51
1:B:254:LEU:HD13	1:B:255:ASP:O	2.10	0.51
1:B:283:PHE:C	1:B:286:PRO:HD2	2.34	0.51
1:A:534:THR:HG23	1:A:538:LEU:HD12	1.92	0.51
1:A:832:LEU:N	1:A:832:LEU:CD1	2.73	0.51
1:A:365:GLU:CD	1:A:368:ARG:HE	2.18	0.51
1:A:408:ILE:HB	1:A:467:LEU:HD13	1.93	0.51
1:B:33:LEU:HB3	1:B:265:GLY:HA3	1.92	0.51
1:B:739:GLU:HA	1:B:744:PHE:HD2	1.71	0.51
1:B:832:LEU:N	1:B:832:LEU:CD1	2.73	0.51
1:A:109:TYR:CD2	1:A:136:HIS:HD2	2.28	0.51
1:A:89:SER:HA	1:A:94:GLU:O	2.11	0.51
1:B:65:ASP:OD2	1:B:68:ASN:HB2	2.11	0.51
1:B:87:ILE:O	1:B:91:THR:HG23	2.10	0.51
1:B:369:GLU:O	1:B:373:GLY:HA3	2.11	0.51
1:B:593:ASN:HB2	1:B:594:HIS:HD2	1.75	0.51
1:A:164:THR:OG1	1:A:796:GLU:OE2	2.29	0.50
1:A:332:MET:HA	1:A:335:GLU:HG3	1.94	0.50
1:A:369:GLU:O	1:A:373:GLY:HA3	2.11	0.50
1:B:164:THR:OG1	1:B:796:GLU:OE2	2.29	0.50
1:B:281:ALA:HB2	1:B:572:ILE:HD11	1.92	0.50
1:A:593:ASN:HB3	1:A:594:HIS:CD2	2.47	0.50
1:B:179:GLU:O	1:B:183:VAL:HG23	2.11	0.50
1:A:179:GLU:O	1:A:183:VAL:HG23	2.11	0.50
1:A:475:HIS:HE1	1:A:477:ASN:ND2	1.96	0.50
1:A:690:MET:CE	1:A:690:MET:CA	2.86	0.50
1:B:251:THR:O	1:B:251:THR:OG1	2.28	0.50
1:B:374:LEU:HD11	1:B:718:GLN:CA	2.38	0.50
1:A:416:THR:CG2	1:A:419:GLU:HB2	2.41	0.50
1:A:65:ASP:OD2	1:A:68:ASN:HB2	2.11	0.50
1:B:71:LYS:O	1:B:173:THR:C	2.52	0.50
1:B:263:ARG:NE	1:B:557:ASN:HD22	2.08	0.50
1:B:416:THR:CG2	1:B:419:GLU:HB2	2.41	0.50
1:B:494:VAL:O	1:B:497:SER:N	2.44	0.50
1:A:284:ILE:CD1	1:A:337:PHE:CE2	2.95	0.50
1:B:416:THR:HG22	1:B:419:GLU:CB	2.40	0.50
1:B:647:ARG:NH1	1:B:694:GLU:OE1	2.35	0.50
1:B:372:ALA:HB2	1:B:630:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD11	1:A:718:GLN:CA	2.39	0.49
1:A:412:LEU:O	1:A:413:ASP:HB2	2.10	0.49
1:A:417:VAL:CG2	1:A:418:GLU:N	2.74	0.49
1:B:352:VAL:HB	1:B:721:VAL:HA	1.94	0.49
1:B:408:ILE:HG22	1:B:467:LEU:HB3	1.94	0.49
1:B:593:ASN:HB3	1:B:594:HIS:CD2	2.47	0.49
1:A:207:ASP:O	1:A:247:ARG:CG	2.61	0.49
1:B:109:TYR:CD2	1:B:136:HIS:HD2	2.28	0.49
1:B:436:MET:HE2	1:B:436:MET:HA	1.94	0.49
1:B:660:ILE:HD11	1:B:693:ARG:HG2	1.92	0.49
1:B:844:SER:OG	1:B:845:GLU:N	2.45	0.49
1:A:352:VAL:HB	1:A:721:VAL:HA	1.94	0.49
1:B:284:ILE:CD1	1:B:337:PHE:CE2	2.95	0.49
1:B:524:HIS:O	1:B:559:ASN:ND2	2.44	0.49
1:A:372:ALA:HB2	1:A:630:PRO:HG2	1.94	0.49
1:A:837:TYR:HE2	1:A:839:LEU:HD12	1.77	0.49
1:B:332:MET:HA	1:B:335:GLU:HG3	1.94	0.49
1:A:63:VAL:HG12	1:A:64:THR:N	2.27	0.49
1:A:470:GLU:HB2	1:A:487:VAL:HG22	1.95	0.49
1:A:498:LEU:HD13	1:A:747:LEU:HD21	1.95	0.49
1:A:602:LEU:HD22	1:A:705:TRP:CH2	2.47	0.49
1:B:660:ILE:HG23	1:B:666:LEU:HD23	1.95	0.49
1:A:119:HIS:CE1	1:A:120:PHE:CD2	3.01	0.49
1:A:385:PHE:CE2	1:A:408:ILE:CD1	2.87	0.49
1:A:646:VAL:O	1:A:650:ILE:HG12	2.13	0.49
1:B:63:VAL:HG12	1:B:64:THR:N	2.27	0.49
1:A:844:SER:OG	1:A:845:GLU:N	2.45	0.49
1:B:493:GLY:O	1:B:496:ASP:HB3	2.13	0.49
1:B:562:ALA:HA	1:B:566:LEU:HB2	1.95	0.49
1:B:778:HIS:NE2	1:B:851:ARG:O	2.45	0.49
1:A:323:SER:OG	1:A:324:ILE:HD12	2.13	0.48
1:B:119:HIS:CE1	1:B:120:PHE:CD2	3.01	0.48
1:B:164:THR:HG23	1:B:546:LYS:CE	2.43	0.48
1:B:323:SER:OG	1:B:324:ILE:HD12	2.13	0.48
1:B:806:PHE:O	1:B:810:VAL:HG23	2.13	0.48
1:A:164:THR:HG23	1:A:546:LYS:CE	2.43	0.48
1:A:374:LEU:CD1	1:A:717:GLY:C	2.87	0.48
1:A:385:PHE:HD1	1:A:385:PHE:C	2.17	0.48
1:B:715:ASN:ND2	1:B:775:LEU:O	2.46	0.48
1:A:593:ASN:C	1:A:594:HIS:CD2	2.92	0.48
1:B:572:ILE:O	1:B:572:ILE:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:PHE:O	1:A:810:VAL:HG23	2.13	0.48
1:B:602:LEU:HD22	1:B:705:TRP:CH2	2.47	0.48
1:A:436:MET:HA	1:A:436:MET:HE2	1.94	0.48
1:A:615:ASP:O	1:A:618:ALA:HB3	2.13	0.48
1:B:470:GLU:HB2	1:B:487:VAL:HG22	1.95	0.48
1:B:646:VAL:O	1:B:650:ILE:HG12	2.13	0.48
1:B:837:TYR:HE2	1:B:839:LEU:HD12	1.77	0.48
1:A:517:ILE:CD1	1:A:590:ILE:HD12	2.42	0.48
1:A:524:HIS:O	1:A:559:ASN:ND2	2.44	0.48
1:A:715:ASN:ND2	1:A:775:LEU:O	2.46	0.48
1:B:207:ASP:O	1:B:247:ARG:CG	2.60	0.48
1:B:469:ILE:HG13	1:B:499:TRP:CH2	2.48	0.48
1:B:593:ASN:C	1:B:594:HIS:CD2	2.92	0.48
1:B:615:ASP:O	1:B:618:ALA:HB3	2.13	0.48
1:A:469:ILE:HG13	1:A:499:TRP:CH2	2.48	0.48
1:A:475:HIS:HB2	1:A:482:GLY:C	2.39	0.48
1:A:660:ILE:HG23	1:A:666:LEU:HD23	1.95	0.48
1:B:374:LEU:CD1	1:B:717:GLY:C	2.87	0.48
1:A:562:ALA:HA	1:A:566:LEU:HB2	1.96	0.48
1:B:516:LEU:HD21	1:B:573:PHE:HE1	1.79	0.48
1:B:692:THR:OG1	1:B:695:GLU:CG	2.53	0.48
1:B:27:LEU:HD22	1:B:123:PHE:CD2	2.49	0.48
1:B:475:HIS:HB2	1:B:482:GLY:C	2.39	0.48
1:B:566:LEU:O	1:B:573:PHE:CB	2.61	0.48
1:A:28:MET:HE2	1:A:33:LEU:HD22	1.95	0.47
1:A:711:HIS:CE1	1:A:859:ILE:O	2.67	0.47
1:B:311:GLU:C	1:B:343:LYS:CB	2.77	0.47
1:B:612:ALA:HB2	1:B:624:LEU:HD23	1.96	0.47
1:B:706:VAL:HA	1:B:710:LEU:HB3	1.97	0.47
1:B:711:HIS:CE1	1:B:859:ILE:O	2.67	0.47
1:A:215:PRO:C	1:A:216:ARG:HD3	2.39	0.47
1:A:405:LYS:HE2	1:A:417:VAL:CG2	2.44	0.47
1:A:550:PRO:HG2	1:A:788:ARG:CZ	2.44	0.47
1:B:413:ASP:N	1:B:413:ASP:OD1	2.46	0.47
1:A:86:THR:O	1:A:89:SER:N	2.47	0.47
1:B:28:MET:HE2	1:B:33:LEU:HD22	1.95	0.47
1:A:321:ILE:C	1:A:323:SER:N	2.65	0.47
1:A:39:ASN:ND2	1:A:40:ALA:N	2.62	0.47
1:A:58:LEU:HD13	1:A:110:PRO:HB3	1.96	0.47
1:B:374:LEU:HD13	1:B:721:VAL:CG2	2.44	0.47
1:B:517:ILE:CD1	1:B:590:ILE:HD12	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PRO:CG	1:B:592:LYS:HB2	2.45	0.47
1:B:698:GLU:O	1:B:702:ILE:HG13	2.15	0.47
1:B:725:LEU:HB3	1:B:726:PRO:CD	2.44	0.47
1:A:27:LEU:HD22	1:A:123:PHE:CD2	2.49	0.47
1:A:119:HIS:CE1	1:A:120:PHE:CE2	3.03	0.47
1:A:306:LEU:CD2	1:A:353:ILE:HD11	2.44	0.47
1:A:602:LEU:HB3	1:A:603:PRO:HD3	1.97	0.47
1:A:605:GLU:OE1	1:A:609:ARG:NE	2.39	0.47
1:A:725:LEU:HB3	1:A:726:PRO:CD	2.44	0.47
1:B:475:HIS:ND1	1:B:476:PRO:HD2	2.30	0.47
1:B:550:PRO:HG2	1:B:788:ARG:CZ	2.44	0.47
1:B:579:PRO:HB2	1:B:583:ALA:HA	1.97	0.47
1:B:142:ILE:HG23	1:B:142:ILE:O	2.15	0.47
1:B:240:GLU:CD	1:B:240:GLU:N	2.73	0.47
1:B:334:LYS:HG2	1:B:339:THR:HG23	1.96	0.47
1:A:226:PRO:CG	1:A:592:LYS:HB2	2.45	0.47
1:A:475:HIS:CE1	1:A:476:PRO:HD2	2.50	0.47
1:A:698:GLU:O	1:A:702:ILE:HG13	2.15	0.47
1:B:135:GLY:C	1:B:136:HIS:ND1	2.73	0.47
1:A:475:HIS:ND1	1:A:476:PRO:HD2	2.30	0.47
1:B:527:ILE:HD13	1:B:527:ILE:HA	1.74	0.47
1:A:135:GLY:C	1:A:136:HIS:ND1	2.73	0.46
1:A:377:VAL:HA	1:A:609:ARG:NH2	2.30	0.46
1:A:612:ALA:HB2	1:A:624:LEU:HD23	1.96	0.46
1:B:475:HIS:CE1	1:B:476:PRO:HD2	2.50	0.46
1:A:413:ASP:OD2	1:A:459:LYS:HE3	2.15	0.46
1:A:579:PRO:HB2	1:A:583:ALA:HA	1.97	0.46
1:A:643:GLU:OE1	1:A:698:GLU:OE1	2.33	0.46
1:B:628:ASP:OD2	1:B:826:LEU:HB3	2.15	0.46
1:B:643:GLU:OE1	1:B:698:GLU:OE1	2.33	0.46
1:B:838:THR:HB	1:B:851:ARG:HB3	1.98	0.46
1:A:847:GLY:O	1:A:849:THR:HG23	2.16	0.46
1:B:415:LEU:HD12	1:B:420:ALA:HA	1.97	0.46
1:B:796:GLU:OE2	1:B:796:GLU:N	2.49	0.46
1:A:352:VAL:O	1:A:833:VAL:HG11	2.16	0.46
1:A:706:VAL:HA	1:A:710:LEU:HB3	1.96	0.46
1:B:58:LEU:HD13	1:B:110:PRO:HB3	1.96	0.46
1:B:83:TRP:HB2	1:B:96:ALA:O	2.15	0.46
1:B:377:VAL:HA	1:B:609:ARG:NH2	2.30	0.46
1:B:593:ASN:HB2	1:B:594:HIS:CD2	2.51	0.46
1:A:25:VAL:HG22	1:A:128:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD13	1:A:721:VAL:CG2	2.44	0.46
1:A:447:THR:HG23	1:A:731:ILE:HG23	1.98	0.46
1:A:565:ILE:HD11	1:A:566:LEU:HD12	1.89	0.46
1:B:254:LEU:HD13	1:B:255:ASP:N	2.31	0.46
1:B:447:THR:HG23	1:B:731:ILE:HG23	1.98	0.46
1:A:508:VAL:HG13	1:A:730:THR:O	2.16	0.46
1:A:164:THR:HG23	1:A:546:LYS:HD2	1.98	0.46
1:B:416:THR:HG22	1:B:419:GLU:HB2	1.97	0.46
1:A:240:GLU:CD	1:A:240:GLU:N	2.73	0.46
1:B:164:THR:HG23	1:B:546:LYS:HD2	1.98	0.46
1:B:514:HIS:HA	1:B:518:SER:HB2	1.98	0.46
1:B:602:LEU:HB3	1:B:603:PRO:HD3	1.97	0.46
1:A:443:ASN:ND2	1:A:448:LYS:HA	2.31	0.46
1:A:628:ASP:OD2	1:A:826:LEU:HB3	2.15	0.46
1:A:796:GLU:OE2	1:A:796:GLU:N	2.49	0.46
1:A:827:LYS:HD3	1:A:827:LYS:H	1.80	0.46
1:B:469:ILE:HD13	1:B:506:VAL:HG11	1.97	0.46
1:B:508:VAL:HG13	1:B:730:THR:O	2.16	0.46
1:A:142:ILE:O	1:A:142:ILE:HG23	2.15	0.46
1:A:514:HIS:HA	1:A:518:SER:HB2	1.98	0.46
1:A:838:THR:HB	1:A:851:ARG:HB3	1.98	0.46
1:B:415:LEU:CG	1:B:419:GLU:HB3	2.46	0.46
1:A:68:ASN:HD21	1:A:74:LEU:HD11	1.72	0.45
1:A:256:ILE:HD11	1:A:563:ARG:NH2	2.25	0.45
1:A:593:ASN:HB2	1:A:594:HIS:CD2	2.51	0.45
1:A:655:LYS:O	1:A:693:ARG:NH1	2.49	0.45
1:B:119:HIS:CE1	1:B:120:PHE:CE2	3.03	0.45
1:B:352:VAL:O	1:B:833:VAL:HG11	2.15	0.45
1:A:633:VAL:HG11	1:A:829:ARG:HH12	1.82	0.45
1:B:25:VAL:HG22	1:B:128:LEU:HD13	1.98	0.45
1:B:847:GLY:O	1:B:849:THR:HG23	2.16	0.45
1:B:39:ASN:ND2	1:B:40:ALA:N	2.62	0.45
1:B:124:LEU:HD12	1:B:125:LEU:N	2.32	0.45
1:B:215:PRO:C	1:B:216:ARG:HD3	2.42	0.45
1:A:43:LEU:C	1:A:43:LEU:CD1	2.85	0.45
1:A:124:LEU:HD12	1:A:125:LEU:N	2.32	0.45
1:B:82:ASP:H	1:B:98:LYS:HB2	1.80	0.45
1:B:288:LEU:HB3	1:B:763:LEU:HD11	1.98	0.45
1:A:258:VAL:HG22	1:A:263:ARG:NH1	2.31	0.45
1:A:469:ILE:HD13	1:A:506:VAL:HG11	1.97	0.45
1:A:288:LEU:HB3	1:A:763:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:ND2	1:A:319:ALA:HB3	2.32	0.45
1:A:491:GLY:O	1:A:496:ASP:HB2	2.17	0.45
1:B:103:TYR:CD1	1:B:103:TYR:C	2.95	0.45
1:A:254:LEU:HD13	1:A:255:ASP:N	2.31	0.45
1:A:778:HIS:NE2	1:A:851:ARG:O	2.45	0.45
1:A:103:TYR:CD1	1:A:103:TYR:C	2.95	0.45
1:A:698:GLU:HA	1:A:701:THR:HG22	1.99	0.45
1:B:59:VAL:HG12	1:B:60:SER:N	2.32	0.45
1:B:258:VAL:HG22	1:B:263:ARG:NH1	2.31	0.45
1:B:317:ASN:ND2	1:B:319:ALA:HB3	2.32	0.45
1:B:691:GLN:HE21	1:B:691:GLN:HB3	1.60	0.45
1:A:371:LEU:HB3	1:A:629:TYR:CD2	2.52	0.45
1:A:634:ASP:O	1:A:638:VAL:HG23	2.17	0.45
1:A:837:TYR:CE2	1:A:839:LEU:HD12	2.52	0.45
1:B:103:TYR:CE1	1:B:104:GLU:O	2.70	0.45
1:B:768:GLY:O	1:B:772:ILE:HG12	2.17	0.45
1:A:827:LYS:N	1:A:827:LYS:CD	2.79	0.44
1:B:98:LYS:HA	1:B:98:LYS:HD3	1.71	0.44
1:B:306:LEU:CD2	1:B:353:ILE:HD11	2.44	0.44
1:B:634:ASP:O	1:B:638:VAL:HG23	2.17	0.44
1:B:176:LYS:O	1:B:180:GLU:HG3	2.18	0.44
1:B:498:LEU:HD12	1:B:747:LEU:HD21	1.97	0.44
1:B:731:ILE:HG22	1:B:732:SER:N	2.32	0.44
1:B:744:PHE:O	1:B:744:PHE:CD1	2.70	0.44
1:A:98:LYS:HD3	1:A:98:LYS:HA	1.71	0.44
1:A:103:TYR:CE1	1:A:104:GLU:O	2.70	0.44
1:B:581:LYS:HE2	3:B:1004:HOH:O	2.13	0.44
1:A:276:ALA:O	1:A:279:ALA:HB3	2.18	0.44
1:A:330:LEU:O	1:A:333:LEU:N	2.50	0.44
1:A:443:ASN:HD22	1:A:443:ASN:HA	1.60	0.44
1:A:567:ILE:HB	1:A:584:MET:SD	2.58	0.44
1:B:415:LEU:HD22	1:B:419:GLU:HG2	1.97	0.44
1:B:315:LEU:HD21	1:B:345:LEU:CD1	2.48	0.44
1:B:383:LYS:HA	1:B:421:LEU:HD23	1.99	0.44
1:B:633:VAL:HG11	1:B:829:ARG:HH12	1.82	0.44
1:A:59:VAL:HG12	1:A:60:SER:N	2.32	0.44
1:A:116:ARG:NH1	1:A:116:ARG:CG	2.73	0.44
1:A:449:THR:HG22	1:A:450:TYR:N	2.26	0.44
1:B:139:VAL:HG22	1:B:141:TYR:CE2	2.52	0.44
1:B:256:ILE:HD11	1:B:563:ARG:NH2	2.25	0.44
1:B:443:ASN:ND2	1:B:448:LYS:HA	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:HG22	1:A:141:TYR:CE2	2.53	0.44
1:A:505:PHE:CZ	1:A:734:GLN:O	2.70	0.44
1:A:731:ILE:HG22	1:A:732:SER:N	2.32	0.44
1:B:68:ASN:HD22	1:B:74:LEU:HD12	1.78	0.44
1:B:344:PHE:CD1	1:B:344:PHE:O	2.70	0.44
1:B:416:THR:CG2	1:B:419:GLU:CB	2.95	0.44
1:B:605:GLU:OE1	1:B:609:ARG:NE	2.39	0.44
1:A:586:MET:HE2	1:A:586:MET:HB3	1.77	0.44
1:B:385:PHE:HA	1:B:386:PRO:C	2.42	0.44
1:A:330:LEU:O	1:A:331:GLU:C	2.61	0.43
1:A:768:GLY:O	1:A:772:ILE:HG12	2.17	0.43
1:B:837:TYR:CE2	1:B:839:LEU:HD12	2.52	0.43
1:A:148:TYR:CZ	1:A:195:GLU:OE2	2.68	0.43
1:A:744:PHE:O	1:A:744:PHE:CD1	2.70	0.43
1:B:44:ASP:O	1:B:45:ARG:HB2	2.18	0.43
1:B:205:TYR:HB2	1:B:219:LEU:HB2	2.00	0.43
1:B:276:ALA:O	1:B:279:ALA:HB3	2.18	0.43
1:B:567:ILE:HB	1:B:584:MET:SD	2.58	0.43
1:B:793:TRP:CD1	1:B:793:TRP:H	2.37	0.43
1:A:263:ARG:NE	1:A:557:ASN:HD22	2.08	0.43
1:A:377:VAL:O	1:A:609:ARG:NE	2.52	0.43
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.78	0.43
1:B:178:ARG:NH2	1:B:665:GLU:OE1	2.51	0.43
1:B:377:VAL:O	1:B:609:ARG:NE	2.52	0.43
1:B:498:LEU:CD1	1:B:747:LEU:CD2	2.96	0.43
1:A:773:GLU:O	1:A:777:THR:HG23	2.19	0.43
1:B:449:THR:HG22	1:B:450:TYR:N	2.26	0.43
1:B:773:GLU:O	1:B:777:THR:HG23	2.19	0.43
1:A:370:MET:SD	1:A:429:LEU:HD22	2.59	0.43
1:A:385:PHE:HA	1:A:386:PRO:C	2.42	0.43
1:B:71:LYS:O	1:B:173:THR:CA	2.67	0.43
1:B:312:GLY:CA	1:B:345:LEU:O	2.66	0.43
1:B:371:LEU:HB3	1:B:629:TYR:CD2	2.52	0.43
1:B:385:PHE:HB2	1:B:421:LEU:HD11	2.00	0.43
1:B:415:LEU:CD1	1:B:419:GLU:HB3	2.48	0.43
1:B:415:LEU:CD1	1:B:420:ALA:CA	2.96	0.43
1:A:205:TYR:HB2	1:A:219:LEU:HB2	2.00	0.43
1:A:849:THR:O	1:A:851:ARG:HG2	2.19	0.43
1:A:405:LYS:CE	1:A:418:GLU:OE2	2.67	0.43
1:A:793:TRP:CD1	1:A:793:TRP:H	2.37	0.43
1:B:630:PRO:HB3	1:B:837:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:GLU:HA	1:B:701:THR:HG22	1.99	0.43
1:A:45:ARG:NH1	1:A:45:ARG:CG	2.73	0.43
1:A:634:ASP:CG	1:A:829:ARG:HH21	2.27	0.43
1:A:411:ASN:HB3	1:A:467:LEU:HD22	2.01	0.43
1:B:320:LEU:O	1:B:324:ILE:CD1	2.67	0.43
1:B:417:VAL:HG23	1:B:418:GLU:N	2.32	0.43
1:B:443:ASN:ND2	1:B:449:THR:H	1.96	0.43
1:B:584:MET:HB3	1:B:584:MET:HE3	1.77	0.43
1:A:25:VAL:HG22	1:A:128:LEU:CD1	2.49	0.42
1:A:660:ILE:CD1	1:A:693:ARG:HG2	2.46	0.42
1:A:732:SER:HA	1:A:758:THR:O	2.19	0.42
1:B:148:TYR:CZ	1:B:195:GLU:OE2	2.68	0.42
1:B:312:GLY:HA2	1:B:345:LEU:O	2.19	0.42
1:B:56:LEU:HA	1:B:114:LEU:O	2.19	0.42
1:B:82:ASP:O	1:B:98:LYS:CB	2.65	0.42
1:B:732:SER:HA	1:B:758:THR:O	2.19	0.42
1:B:801:GLU:O	1:B:805:LYS:HG2	2.19	0.42
1:A:348:PRO:O	1:A:350:PRO:HD3	2.20	0.42
1:B:25:VAL:HG22	1:B:128:LEU:CD1	2.49	0.42
1:A:56:LEU:HA	1:A:114:LEU:O	2.19	0.42
1:A:71:LYS:O	1:A:173:THR:CA	2.67	0.42
1:A:320:LEU:O	1:A:324:ILE:CD1	2.67	0.42
1:A:405:LYS:HE2	1:A:417:VAL:HG22	2.00	0.42
1:B:321:ILE:C	1:B:323:SER:N	2.65	0.42
1:B:464:LEU:HD21	1:B:626:ILE:CD1	2.49	0.42
1:B:736:MET:HE2	1:B:736:MET:HB3	1.82	0.42
1:A:328:ILE:HA	1:A:329:PRO:HD2	1.80	0.42
1:B:194:LYS:HE2	1:B:194:LYS:HB2	1.82	0.42
1:B:348:PRO:O	1:B:350:PRO:HD3	2.20	0.42
1:B:370:MET:SD	1:B:429:LEU:HD22	2.59	0.42
1:A:44:ASP:O	1:A:45:ARG:HB2	2.18	0.42
1:A:402:THR:CG2	1:A:485:SER:HB2	2.49	0.42
1:A:584:MET:HE3	1:A:584:MET:HB3	1.77	0.42
1:B:338:ARG:HB2	1:B:346:LYS:HG2	2.02	0.42
1:B:416:THR:O	1:B:419:GLU:HB2	2.19	0.42
1:A:215:PRO:O	1:A:216:ARG:HD2	2.20	0.42
1:A:528:GLU:HB3	1:A:529:PRO:HD3	2.02	0.42
1:A:801:GLU:O	1:A:805:LYS:HG2	2.19	0.42
1:B:402:THR:CG2	1:B:485:SER:HB2	2.49	0.42
1:B:43:LEU:C	1:B:43:LEU:CD1	2.85	0.42
1:B:457:PHE:HB2	1:B:467:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:LYS:CA	1:B:689:LYS:CE	2.92	0.42
1:B:809:LYS:HE3	1:B:813:ILE:HD11	2.02	0.42
1:A:361:ARG:NH2	1:A:500:GLN:HG2	2.35	0.42
1:A:457:PHE:HB2	1:A:467:LEU:HD11	2.02	0.42
1:A:809:LYS:HE3	1:A:813:ILE:HD11	2.02	0.42
1:B:128:LEU:HB3	1:B:141:TYR:HB2	2.02	0.42
1:B:832:LEU:H	1:B:832:LEU:CD1	2.33	0.42
1:B:849:THR:O	1:B:851:ARG:HG2	2.19	0.42
1:A:207:ASP:OD1	1:A:207:ASP:N	2.50	0.42
1:A:271:ASP:CG	1:A:779:SER:HG	2.28	0.42
1:A:360:TRP:NE1	1:A:724:TYR:HE1	2.18	0.42
1:A:630:PRO:HB3	1:A:837:TYR:CD1	2.54	0.42
1:B:827:LYS:N	1:B:827:LYS:CD	2.79	0.42
1:A:178:ARG:NH2	1:A:665:GLU:OE1	2.51	0.41
1:A:832:LEU:H	1:A:832:LEU:CD1	2.33	0.41
1:A:464:LEU:HD21	1:A:626:ILE:CD1	2.50	0.41
1:B:284:ILE:HD11	1:B:337:PHE:CE2	2.55	0.41
1:B:360:TRP:NE1	1:B:724:TYR:HE1	2.19	0.41
1:B:361:ARG:NH2	1:B:500:GLN:HG2	2.35	0.41
1:B:501:LEU:HD23	1:B:501:LEU:HA	1.84	0.41
1:A:291:VAL:HG13	1:A:316:PRO:HD3	2.02	0.41
1:A:736:MET:HE2	1:A:736:MET:HB3	1.82	0.41
1:B:271:ASP:CG	1:B:779:SER:HG	2.28	0.41
1:A:68:ASN:HD22	1:A:74:LEU:HD12	1.78	0.41
1:A:176:LYS:O	1:A:180:GLU:HG3	2.20	0.41
1:A:284:ILE:HD11	1:A:337:PHE:CE2	2.55	0.41
1:B:553:ARG:HE	1:B:553:ARG:HB2	1.65	0.41
1:A:607:LYS:HE2	1:A:614:GLU:OE2	2.19	0.41
1:A:660:ILE:HD12	1:A:693:ARG:CA	2.42	0.41
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.73	0.41
1:B:494:VAL:O	1:B:497:SER:HB2	2.21	0.41
1:B:573:PHE:O	1:B:577:VAL:CG2	2.48	0.41
1:B:827:LYS:HD3	1:B:827:LYS:H	1.80	0.41
1:A:63:VAL:CG1	1:A:64:THR:N	2.83	0.41
1:A:128:LEU:HB3	1:A:141:TYR:HB2	2.02	0.41
1:A:553:ARG:HE	1:A:553:ARG:HB2	1.65	0.41
1:A:689:LYS:HE2	1:A:689:LYS:CA	2.39	0.41
1:A:517:ILE:N	1:A:517:ILE:HD13	2.36	0.41
1:A:527:ILE:HA	1:A:527:ILE:HD13	1.74	0.41
1:A:71:LYS:O	1:A:173:THR:HB	2.21	0.41
1:A:258:VAL:HG22	1:A:263:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LYS:HD2	1:A:448:LYS:N	2.32	0.41
1:A:494:VAL:CG1	1:A:495:TYR:N	2.83	0.41
1:A:778:HIS:HB2	1:A:847:GLY:O	2.20	0.41
1:B:283:PHE:O	1:B:286:PRO:HD2	2.21	0.41
1:B:503:LYS:HB2	1:B:503:LYS:HE3	1.94	0.41
1:B:505:PHE:CZ	1:B:734:GLN:O	2.70	0.41
1:B:757:LYS:HB3	1:B:757:LYS:HE3	1.83	0.41
1:A:50:LEU:HD21	1:A:82:ASP:HA	2.02	0.41
1:B:63:VAL:CG1	1:B:64:THR:N	2.83	0.41
1:B:71:LYS:O	1:B:173:THR:HB	2.21	0.41
1:B:258:VAL:HG22	1:B:263:ARG:CZ	2.51	0.41
1:B:276:ALA:O	1:B:280:ILE:HG13	2.21	0.41
1:B:291:VAL:HG13	1:B:316:PRO:HD3	2.02	0.41
1:B:521:MET:O	1:B:526:SER:OG	2.25	0.41
1:B:721:VAL:HG12	1:B:835:MET:HE1	2.03	0.41
1:B:725:LEU:HD22	1:B:765:THR:OG1	2.21	0.41
1:B:778:HIS:HB2	1:B:847:GLY:O	2.20	0.41
1:A:166:LEU:H	1:A:169:GLU:CG	2.33	0.40
1:B:22:LYS:HE2	1:B:22:LYS:HB2	1.89	0.40
1:B:45:ARG:NH1	1:B:45:ARG:CG	2.73	0.40
1:B:528:GLU:HB3	1:B:529:PRO:HD3	2.02	0.40
1:A:517:ILE:HG23	1:A:521:MET:CE	2.51	0.40
1:A:522:GLN:CD	3:A:1001:HOH:O	2.64	0.40
1:B:328:ILE:HA	1:B:329:PRO:HD2	1.80	0.40
1:B:517:ILE:HD13	1:B:517:ILE:N	2.36	0.40
1:B:675:GLU:HA	1:B:682:LYS:HE2	2.03	0.40
1:A:565:ILE:CD1	1:A:566:LEU:CD1	2.86	0.40
1:B:35:PHE:HD1	1:B:35:PHE:HA	1.78	0.40
1:B:404:THR:OG1	1:B:407:HIS:ND1	2.49	0.40
1:A:572:ILE:O	1:A:572:ILE:HG22	2.21	0.40
1:A:675:GLU:HA	1:A:682:LYS:HE2	2.04	0.40
1:B:48:GLU:C	1:B:50:LEU:H	2.29	0.40
1:B:166:LEU:H	1:B:169:GLU:CG	2.34	0.40
1:B:263:ARG:HH11	1:B:263:ARG:HD2	1.75	0.40
1:B:516:LEU:CD2	1:B:573:PHE:HE1	2.34	0.40
1:B:579:PRO:HB2	1:B:583:ALA:CA	2.52	0.40
1:A:48:GLU:C	1:A:50:LEU:H	2.29	0.40
1:A:276:ALA:O	1:A:280:ILE:HG13	2.21	0.40
1:A:579:PRO:HB2	1:A:583:ALA:CA	2.52	0.40
1:A:730:THR:HB	1:A:731:ILE:HG13	2.03	0.40
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ASN:HD22	1:B:443:ASN:HA	1.60	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:GLN:CG	1:B:190:GLU:OE1[2_384]	1.87	0.33
1:A:211:PRO:O	1:B:85:THR:O[4_488]	1.99	0.21

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	842/859 (98%)	823 (98%)	19 (2%)	0	100	100
1	B	842/859 (98%)	822 (98%)	20 (2%)	0	100	100
All	All	1684/1718 (98%)	1645 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	745/759 (98%)	630 (85%)	115 (15%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	745/759 (98%)	641 (86%)	104 (14%)	3	15
All	All	1490/1518 (98%)	1271 (85%)	219 (15%)	3	13

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

Mol	Chain	Res	Type
1	A	29	LYS
1	A	31	ASN
1	A	33	LEU
1	A	35	PHE
1	A	37	ASP
1	A	43	LEU
1	A	45	ARG
1	A	46	LEU
1	A	48	GLU
1	A	50	LEU
1	A	53	LYS
1	A	64	THR
1	A	67	GLU
1	A	70	SER
1	A	71	LYS
1	A	86	THR
1	A	89	SER
1	A	91	THR
1	A	95	SER
1	A	102	ASP
1	A	106	ASP
1	A	116	ARG
1	A	139	VAL
1	A	143	CYS
1	A	145	SER
1	A	164	THR
1	A	188	THR
1	A	190	GLU
1	A	194	LYS
1	A	208	LEU
1	A	210	VAL
1	A	213	LYS
1	A	214	ASN
1	A	223	GLN
1	A	236	LYS
1	A	238	THR

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Mol	Chain	Res	Type
1	A	239	LYS
1	A	246	SER
1	A	250	ILE
1	A	253	SER
1	A	254	LEU
1	A	256	ILE
1	A	268	LYS
1	A	270	SER
1	A	284	ILE
1	A	285	GLN
1	A	288	LEU
1	A	294	ASP
1	A	298	GLU
1	A	300	ASP
1	A	322	ASP
1	A	324	ILE
1	A	326	LYS
1	A	330	LEU
1	A	333	LEU
1	A	340	ASP
1	A	342	GLN
1	A	364	GLU
1	A	376	PRO
1	A	378	VAL
1	A	379	ILE
1	A	380	GLN
1	A	381	LEU
1	A	384	GLU
1	A	385	PHE
1	A	401	SER
1	A	402	THR
1	A	404	THR
1	A	405	LYS
1	A	408	ILE
1	A	416	THR
1	A	419	GLU
1	A	421	LEU
1	A	422	GLU
1	A	423	LYS
1	A	424	GLU
1	A	436	MET
1	A	443	ASN

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Mol	Chain	Res	Type
1	A	448	LYS
1	A	464	LEU
1	A	465	LYS
1	A	492	GLU
1	A	498	LEU
1	A	540	VAL
1	A	566	LEU
1	A	576	THR
1	A	577	VAL
1	A	578	PHE
1	A	590	ILE
1	A	594	HIS
1	A	613	VAL
1	A	614	GLU
1	A	617	GLU
1	A	619	PRO
1	A	627	LYS
1	A	689	LYS
1	A	690	MET
1	A	691	GLN
1	A	730	THR
1	A	734	GLN
1	A	736	MET
1	A	740	ASN
1	A	745	GLU
1	A	758	THR
1	A	759	ILE
1	A	760	THR
1	A	825	THR
1	A	826	LEU
1	A	827	LYS
1	A	829	ARG
1	A	830	THR
1	A	833	VAL
1	A	843	SER
1	A	845	GLU
1	A	848	VAL
1	B	29	LYS
1	B	31	ASN
1	B	33	LEU
1	B	35	PHE
1	B	37	ASP

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Mol	Chain	Res	Type
1	B	43	LEU
1	B	45	ARG
1	B	46	LEU
1	B	48	GLU
1	B	50	LEU
1	B	53	LYS
1	B	64	THR
1	B	67	GLU
1	B	70	SER
1	B	71	LYS
1	B	88	THR
1	B	90	LEU
1	B	91	THR
1	B	102	ASP
1	B	106	ASP
1	B	116	ARG
1	B	139	VAL
1	B	143	CYS
1	B	145	SER
1	B	164	THR
1	B	188	THR
1	B	190	GLU
1	B	194	LYS
1	B	213	LYS
1	B	223	GLN
1	B	236	LYS
1	B	238	THR
1	B	239	LYS
1	B	246	SER
1	B	250	ILE
1	B	253	SER
1	B	254	LEU
1	B	256	ILE
1	B	268	LYS
1	B	270	SER
1	B	284	ILE
1	B	285	GLN
1	B	288	LEU
1	B	294	ASP
1	B	298	GLU
1	B	300	ASP
1	B	322	ASP

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Mol	Chain	Res	Type
1	B	324	ILE
1	B	326	LYS
1	B	333	LEU
1	B	342	GLN
1	B	364	GLU
1	B	376	PRO
1	B	378	VAL
1	B	379	ILE
1	B	380	GLN
1	B	381	LEU
1	B	384	GLU
1	B	385	PHE
1	B	401	SER
1	B	402	THR
1	B	404	THR
1	B	405	LYS
1	B	415	LEU
1	B	416	THR
1	B	418	GLU
1	B	421	LEU
1	B	436	MET
1	B	443	ASN
1	B	448	LYS
1	B	464	LEU
1	B	465	LYS
1	B	492	GLU
1	B	498	LEU
1	B	540	VAL
1	B	566	LEU
1	B	576	THR
1	B	577	VAL
1	B	578	PHE
1	B	590	ILE
1	B	594	HIS
1	B	613	VAL
1	B	617	GLU
1	B	619	PRO
1	B	627	LYS
1	B	690	MET
1	B	691	GLN
1	B	730	THR
1	B	734	GLN

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Mol	Chain	Res	Type
1	B	736	MET
1	B	740	ASN
1	B	745	GLU
1	B	758	THR
1	B	759	ILE
1	B	760	THR
1	B	825	THR
1	B	826	LEU
1	B	827	LYS
1	B	829	ARG
1	B	830	THR
1	B	833	VAL
1	B	843	SER
1	B	845	GLU
1	B	848	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	52	ASN
1	A	68	ASN
1	A	79	HIS
1	A	168	HIS
1	A	285	GLN
1	A	342	GLN
1	A	380	GLN
1	A	443	ASN
1	A	477	ASN
1	A	500	GLN
1	A	509	ASN
1	A	535	ASN
1	A	557	ASN
1	A	593	ASN
1	A	594	HIS
1	A	828	ASN
1	B	39	ASN
1	B	52	ASN
1	B	68	ASN
1	B	79	HIS
1	B	168	HIS
1	B	285	GLN

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Mol	Chain	Res	Type
1	B	342	GLN
1	B	380	GLN
1	B	443	ASN
1	B	477	ASN
1	B	500	GLN
1	B	509	ASN
1	B	535	ASN
1	B	557	ASN
1	B	593	ASN
1	B	594	HIS
1	B	691	GLN
1	B	828	ASN

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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	844/859 (98%)	0.16	7 (0%) 82 68	32, 53, 86, 126	0
1	B	844/859 (98%)	0.29	16 (1%) 66 48	36, 58, 91, 126	0
All	All	1688/1718 (98%)	0.23	23 (1%) 73 54	32, 55, 89, 126	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ASN	3.9
1	A	69	GLY	3.0
1	A	47	HIS	3.0
1	B	301	SER	2.8
1	B	417	VAL	2.8
1	B	305	VAL	2.7
1	A	240	GLU	2.7
1	B	317	ASN	2.7
1	B	168	HIS	2.6
1	A	322	ASP	2.5
1	A	43	LEU	2.4
1	B	573	PHE	2.4
1	B	321	ILE	2.3
1	B	393	SER	2.3
1	B	683	SER	2.2
1	B	68	ASN	2.2
1	B	51	GLY	2.1
1	A	340	ASP	2.1
1	B	181	GLU	2.1
1	B	322	ASP	2.1
1	B	776	SER	2.0
1	B	339	THR	2.0
1	B	302	PHE	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($\text{\AA}^2$)	Q<0.9
2	FE	A	901	1/1	0.99	0.09	35,35,35,35	0
2	FE	B	901	1/1	0.99	0.09	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.