Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2024 – 04:18 PM JST

PDB ID	:	8X8F
Title	:	Crystal structure of lipoxygenase from Enhygromyxa salina
Authors	:	Kim, J.W.; Seo, P.W.; Kim, J.S.
Deposited on	:	2023-11-27
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

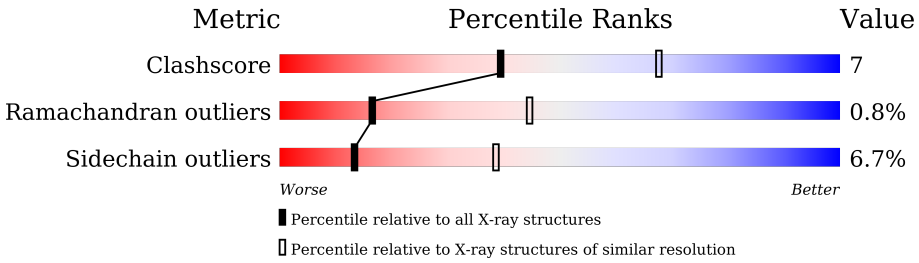
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	650	70% 21% • 7%
1	B	650	74% 16% • 8%
1	C	650	75% 16% • 7%
1	D	650	74% 17% • 7%
1	E	650	75% 15% • 7%
1	F	650	78% 13% • 7%
1	G	650	72% 17% • 7%
1	H	650	76% 16% • 7%

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Mol	Chain	Length	Quality of chain
1	I	650	74% 17% • 7%
1	J	650	75% 15% • 7%
1	K	650	74% 17% • 8%
1	L	650	75% 16% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 56680 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 Arachidonate 15-lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4666	2974	802	879	11			
1	B	600	Total	C	N	O	S	0	0	0
			4615	2946	790	868	11			
1	C	602	Total	C	N	O	S	0	0	0
			4629	2954	792	872	11			
1	D	607	Total	C	N	O	S	0	0	0
			4677	2983	801	882	11			
1	E	604	Total	C	N	O	S	0	0	0
			4650	2966	797	876	11			
1	F	605	Total	C	N	O	S	0	0	0
			4657	2969	798	879	11			
1	G	603	Total	C	N	O	S	0	0	0
			4637	2955	797	874	11			
1	H	604	Total	C	N	O	S	0	0	0
			4646	2963	796	876	11			
1	I	603	Total	C	N	O	S	0	0	0
			4637	2958	794	874	11			
1	J	604	Total	C	N	O	S	0	0	0
			4651	2969	797	874	11			
1	K	600	Total	C	N	O	S	0	0	0
			4612	2944	788	869	11			
1	L	600	Total	C	N	O	S	0	0	0
			4605	2939	787	868	11			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cd	0	0
			4	4		
2	B	4	Total	Cd	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	4	Total Cd 4 4	0	0
2	D	4	Total Cd 4 4	0	0
2	E	4	Total Cd 4 4	0	0
2	F	4	Total Cd 4 4	0	0
2	G	4	Total Cd 4 4	0	0
2	H	4	Total Cd 4 4	0	0
2	I	4	Total Cd 4 4	0	0
2	J	4	Total Cd 4 4	0	0
2	K	4	Total Cd 4 4	0	0
2	L	4	Total Cd 4 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	83	Total O 83 83	0	0
3	B	56	Total O 56 56	0	0
3	C	89	Total O 89 89	0	0
3	D	103	Total O 103 103	0	0
3	E	103	Total O 103 103	0	0
3	F	75	Total O 75 75	0	0
3	G	82	Total O 82 82	0	0
3	H	69	Total O 69 69	0	0
3	I	62	Total O 62 62	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	56	Total O 56 56	0	0
3	K	79	Total O 79 79	0	0
3	L	93	Total O 93 93	0	0

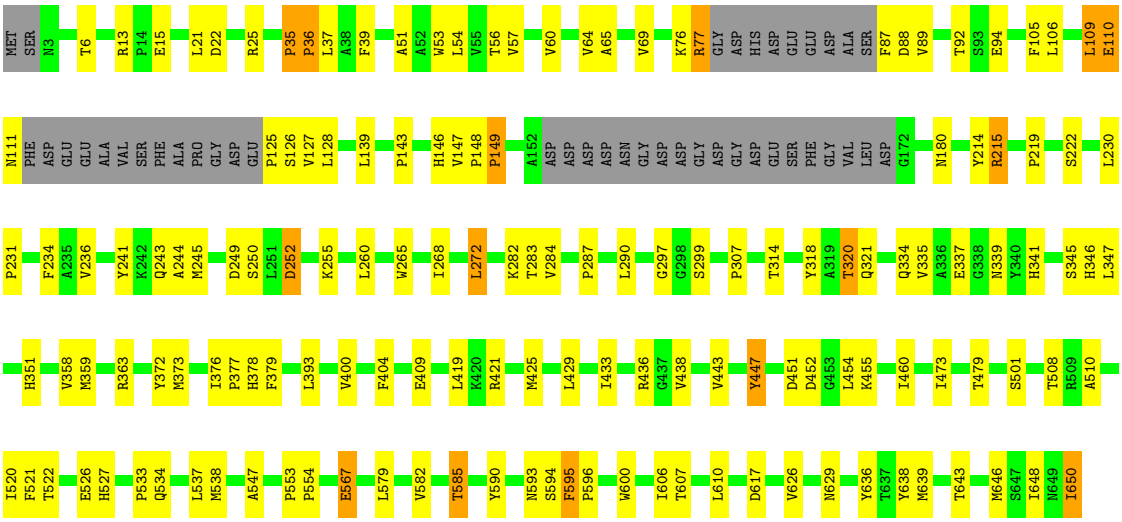
3 Residue-property plots (i)

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

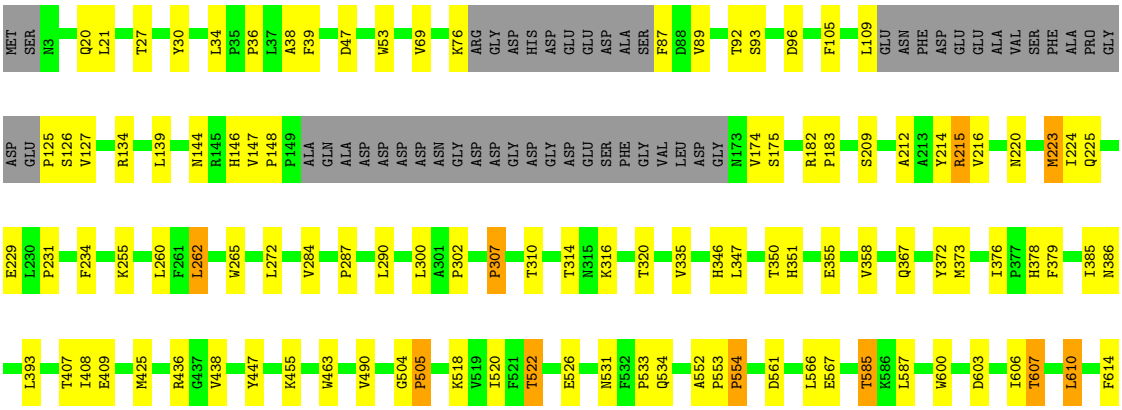
• Molecule 1: Arachidonate 15-lipoxygenase

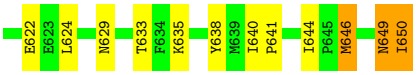
Chain A:



• Molecule 1: Arachidonate 15-lipoxygenase

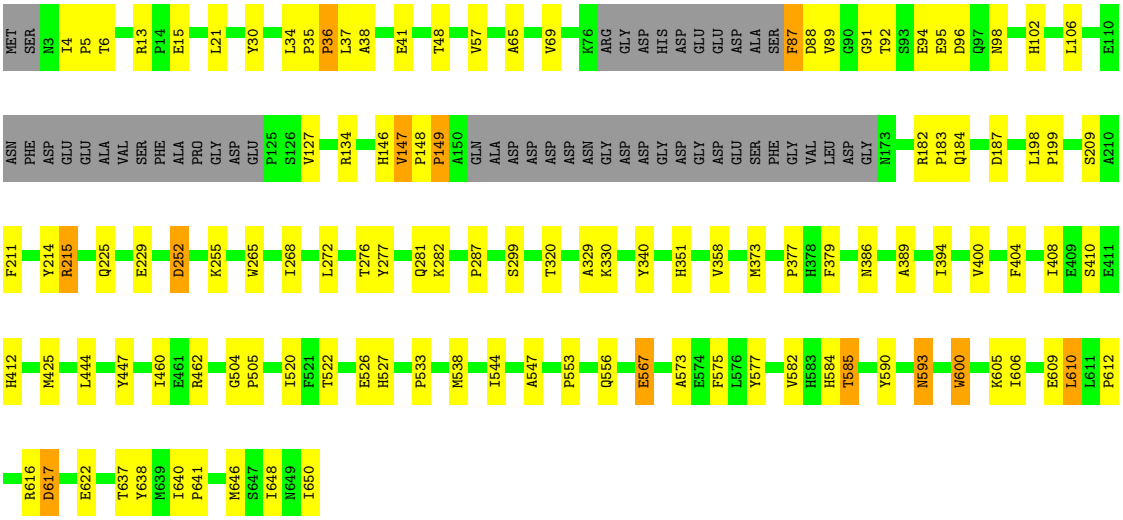
Chain B:





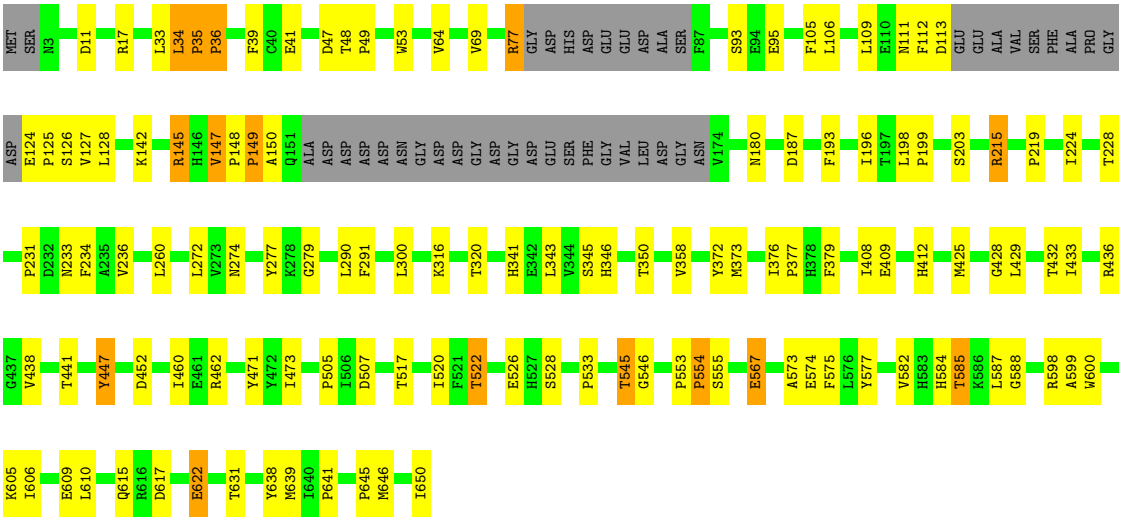
• Molecule 1: Arachidonate 15-lipoxygenase

Chain C:



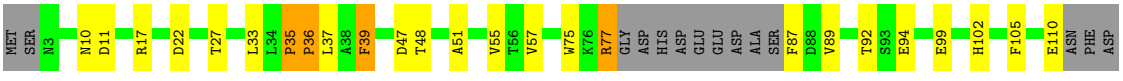
• Molecule 1: Arachidonate 15-lipoxygenase

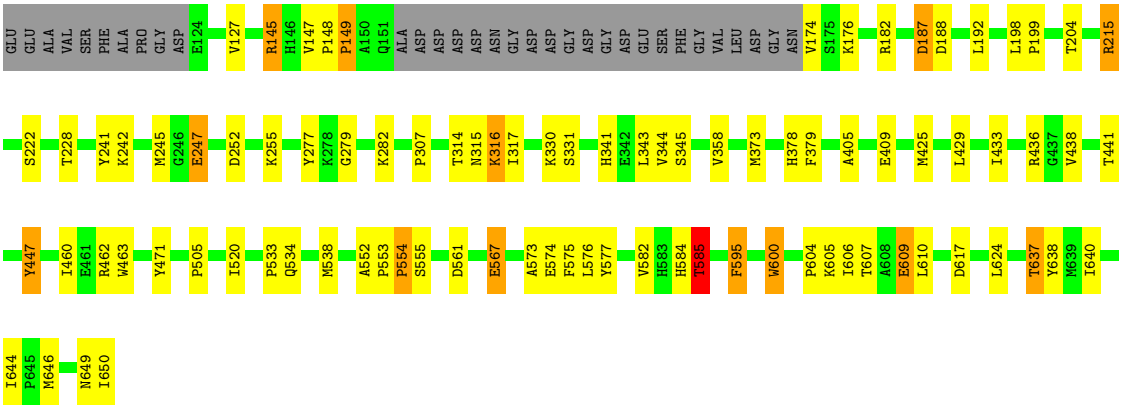
Chain D:



• Molecule 1: Arachidonate 15-lipoxygenase

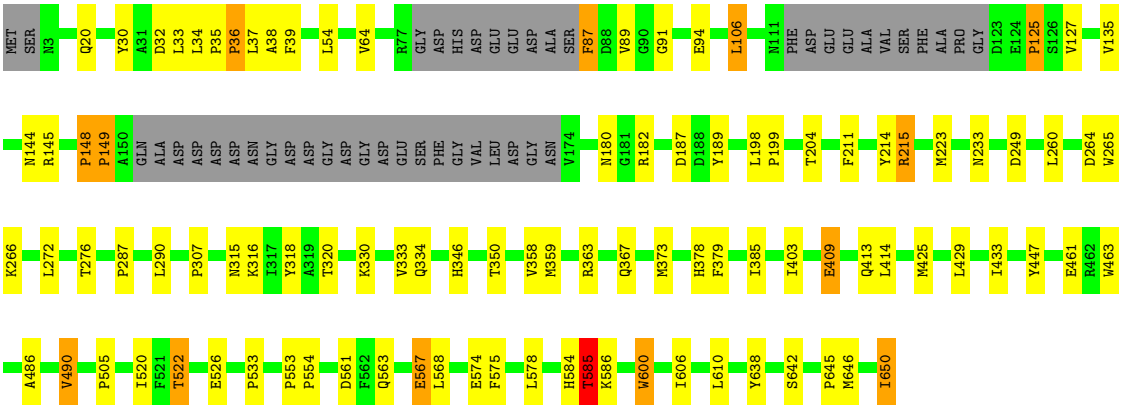
Chain E:





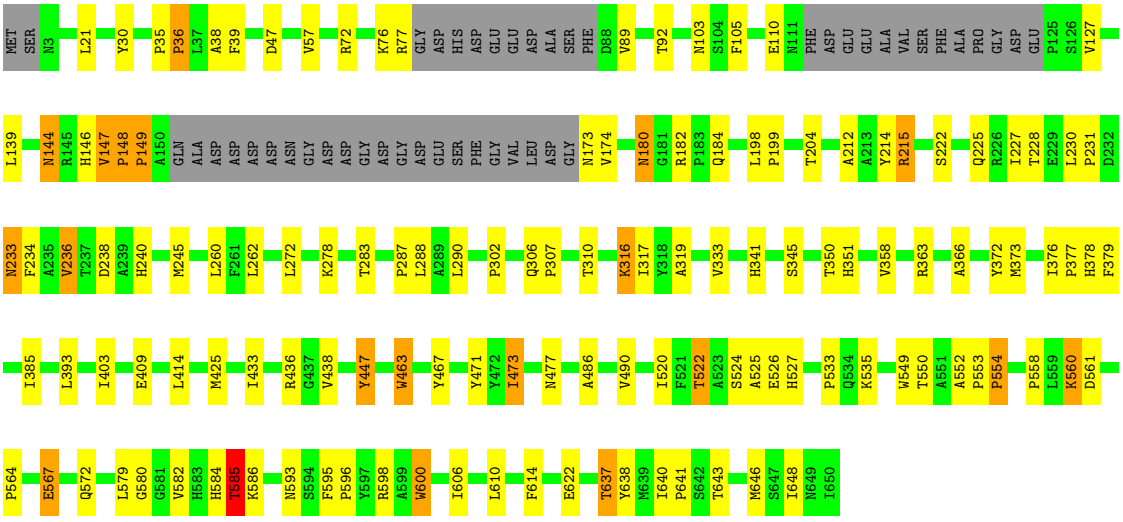
• Molecule 1: Arachidonate 15-lipoxygenase

Chain F:



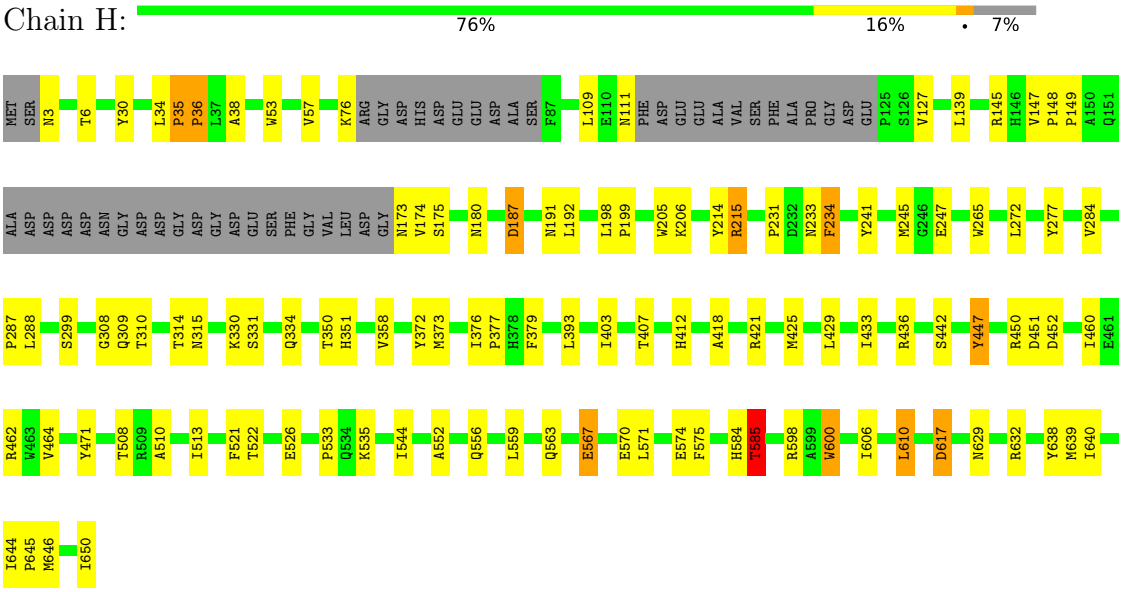
• Molecule 1: Arachidonate 15-lipoxygenase

Chain G:



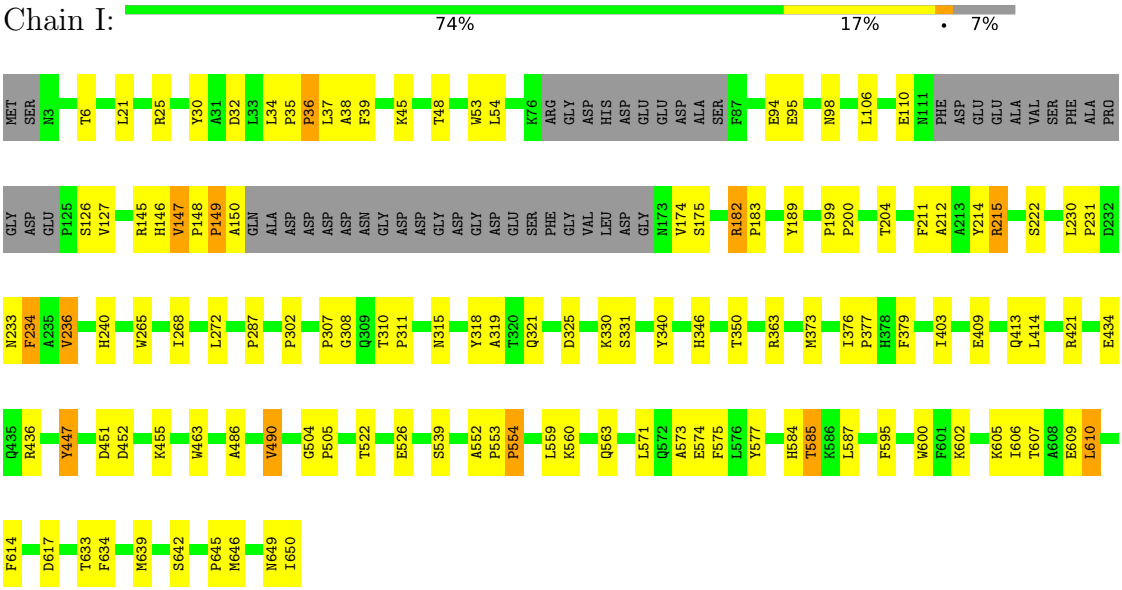
• Molecule 1: Arachidonate 15-lipoxygenase

Chain H:



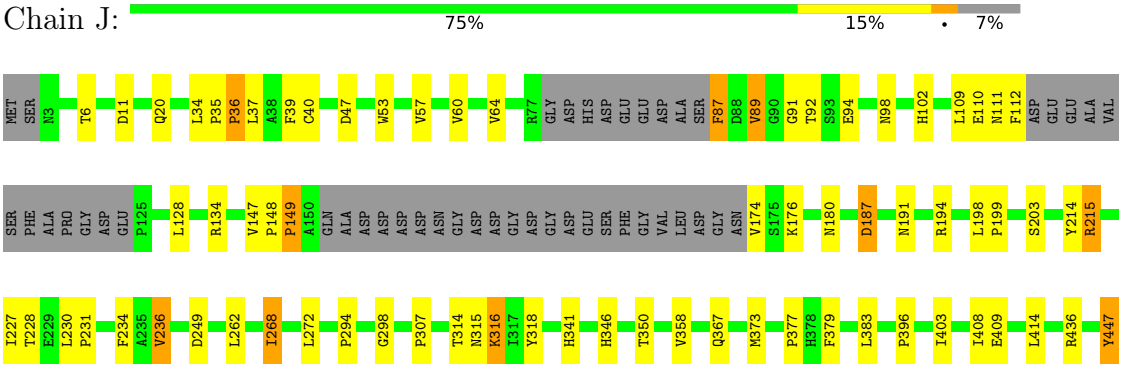
• Molecule 1: Arachidonate 15-lipoxygenase

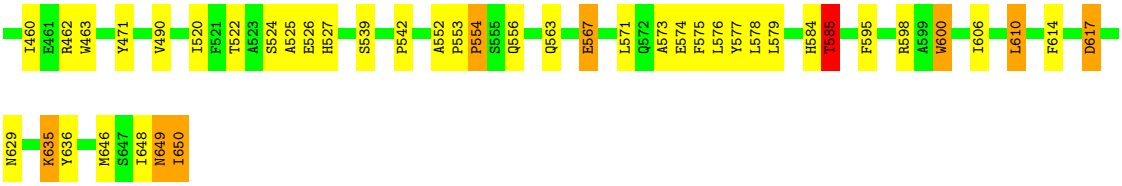
Chain I:



• Molecule 1: Arachidonate 15-lipoxygenase

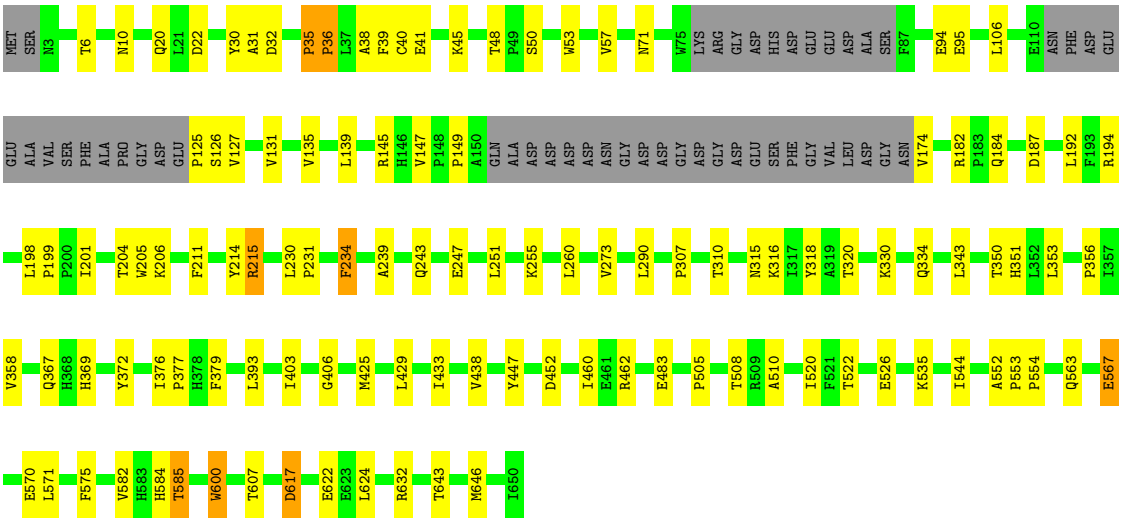
Chain J:





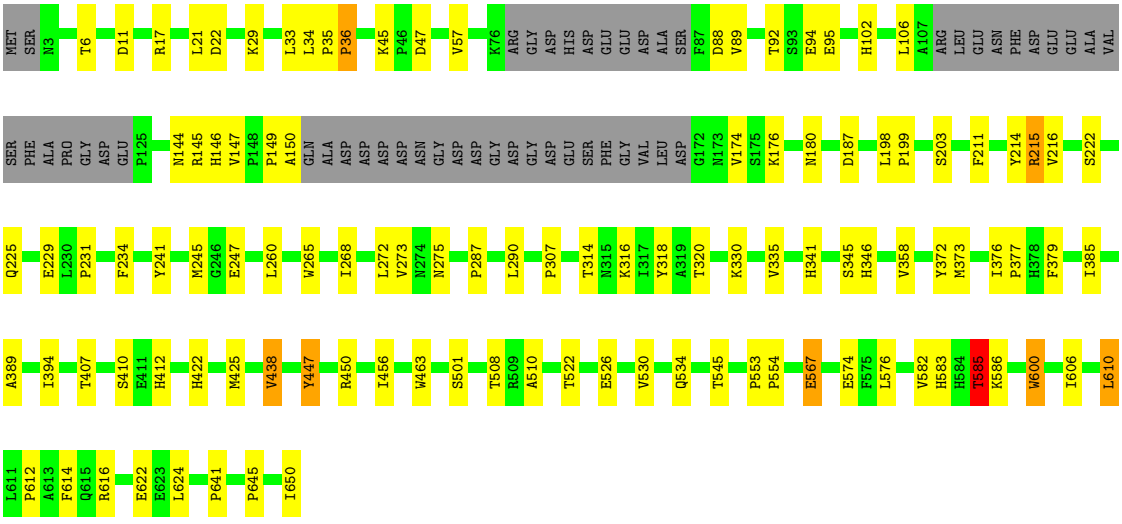
• Molecule 1: Arachidonate 15-lipoxygenase

Chain K:



• Molecule 1: Arachidonate 15-lipoxygenase

Chain L:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	164.73Å 248.59Å 164.09Å 90.00° 119.86° 90.00°	Depositor
Resolution (Å)	49.61 – 2.80	Depositor
% Data completeness (in resolution range)	91.9 (49.61-2.80)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.227 , 0.254	Depositor
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.534	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.145 for l,k,-h-l 0.145 for -h-l,k,h 0.418 for -h-l,-k,l 0.124 for h,-k,-h-l 0.176 for l,-k,h	Xtriage
Total number of atoms	56680	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/4787	0.43	0/6535
1	B	0.26	0/4736	0.43	1/6467 (0.0%)
1	C	0.26	0/4750	0.43	0/6486
1	D	0.26	0/4799	0.43	0/6552
1	E	0.26	0/4771	0.43	0/6514
1	F	0.26	0/4778	0.42	0/6524
1	G	0.26	0/4757	0.43	0/6495
1	H	0.26	0/4767	0.43	0/6509
1	I	0.25	0/4758	0.42	0/6497
1	J	0.26	0/4773	0.43	0/6516
1	K	0.26	0/4733	0.43	0/6464
1	L	0.26	0/4726	0.42	0/6454
All	All	0.26	0/57135	0.43	1/78013 (0.0%)

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	D	0	1
1	E	0	1
1	H	0	2
1	K	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	96	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	PRO	Peptide
1	D	35	PRO	Peptide
1	E	35	PRO	Peptide
1	H	35	PRO	Peptide
1	H	552	ALA	Peptide
1	K	35	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4666	0	4577	77	0
1	B	4615	0	4531	60	0
1	C	4629	0	4542	56	0
1	D	4677	0	4581	64	0
1	E	4650	0	4562	57	0
1	F	4657	0	4564	49	0
1	G	4637	0	4552	67	0
1	H	4646	0	4556	58	0
1	I	4637	0	4548	63	0
1	J	4651	0	4564	69	0
1	K	4612	0	4523	58	0
1	L	4605	0	4515	57	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	83	0	0	0	0
3	B	56	0	0	0	0
3	C	89	0	0	0	0
3	D	103	0	0	0	0
3	E	103	0	0	1	0
3	F	75	0	0	0	0
3	G	82	0	0	1	0
3	H	69	0	0	1	0
3	I	62	0	0	0	0
3	J	56	0	0	0	0
3	K	79	0	0	1	0
3	L	93	0	0	0	0
All	All	56680	0	54615	730	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 7.

All (730) 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:G:148:PRO:HB2	1:G:149:PRO:HD2	1.54	0.89
1:D:148:PRO:HB2	1:D:149:PRO:HD2	1.57	0.87
1:I:585:THR:HG23	1:I:646:MET:H	1.40	0.86
1:B:385:ILE:HG12	1:B:650:ILE:HA	1.58	0.86
1:D:585:THR:HG23	1:D:646:MET:H	1.45	0.82
1:J:148:PRO:HB2	1:J:149:PRO:HD2	1.62	0.81
1:J:35:PRO:O	1:J:37:LEU:N	2.14	0.79
1:E:585:THR:HG23	1:E:646:MET:H	1.48	0.79
1:H:585:THR:HG23	1:H:646:MET:H	1.47	0.78
1:B:585:THR:HG23	1:B:646:MET:H	1.46	0.78
1:G:585:THR:HG23	1:G:646:MET:H	1.46	0.77
1:A:522:THR:HA	1:A:526:GLU:HB3	1.64	0.77
1:B:220:ASN:HD21	1:B:223:MET:HG3	1.50	0.76
1:C:585:THR:HG23	1:C:646:MET:H	1.50	0.76
1:A:585:THR:HG23	1:A:646:MET:H	1.50	0.75
1:E:148:PRO:HB2	1:E:149:PRO:HD2	1.69	0.75
1:K:585:THR:HG23	1:K:646:MET:H	1.50	0.75
1:K:522:THR:HA	1:K:526:GLU:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:ASP:OD2	1:L:17:ARG:NH1	2.20	0.74
1:F:585:THR:HG23	1:F:646:MET:H	1.52	0.74
1:A:148:PRO:HB2	1:A:149:PRO:HD2	1.69	0.74
1:D:522:THR:HA	1:D:526:GLU:HB3	1.70	0.73
1:K:31:ALA:HB2	1:K:41:GLU:HG2	1.71	0.73
1:G:552:ALA:HB1	1:G:554:PRO:HD2	1.71	0.72
1:D:587:LEU:HA	1:D:646:MET:HG2	1.70	0.72
1:A:92:THR:HG23	1:A:147:VAL:HG23	1.72	0.72
1:E:252:ASP:HA	1:E:255:LYS:HE3	1.71	0.72
1:C:148:PRO:HB2	1:C:149:PRO:HD2	1.71	0.72
1:A:436:ARG:NH2	1:A:447:TYR:OH	2.22	0.71
1:K:35:PRO:HB2	1:K:36:PRO:HD2	1.74	0.70
1:I:346:HIS:O	1:I:350:THR:OG1	2.11	0.69
1:F:148:PRO:HB2	1:F:149:PRO:HD2	1.75	0.69
1:I:522:THR:HA	1:I:526:GLU:HB3	1.75	0.68
1:G:522:THR:HA	1:G:526:GLU:HB3	1.75	0.68
1:H:522:THR:HA	1:H:526:GLU:HB3	1.76	0.68
1:G:307:PRO:HB3	1:G:553:PRO:HG2	1.74	0.68
1:J:522:THR:HA	1:J:526:GLU:HB3	1.76	0.68
1:B:182:ARG:HH22	1:B:561:ASP:HA	1.59	0.67
1:H:35:PRO:HB2	1:H:36:PRO:HD2	1.77	0.67
1:K:71:ASN:HA	1:K:194:ARG:HE	1.60	0.67
1:G:230:LEU:HD11	1:G:236:VAL:HG22	1.77	0.67
1:G:436:ARG:NH2	1:G:447:TYR:OH	2.28	0.67
1:J:272:LEU:HD11	1:J:414:LEU:HD22	1.77	0.67
1:I:240:HIS:HD2	1:I:319:ALA:HB2	1.60	0.66
1:D:436:ARG:NH2	1:D:447:TYR:OH	2.27	0.66
1:C:522:THR:HA	1:C:526:GLU:HB3	1.77	0.66
1:J:373:MET:HA	1:J:600:TRP:HZ3	1.61	0.66
1:D:433:ILE:HG23	1:D:438:VAL:HG23	1.77	0.65
1:I:34:LEU:HD23	1:I:37:LEU:HD12	1.78	0.65
1:G:272:LEU:HD11	1:G:414:LEU:HD22	1.78	0.65
1:B:587:LEU:HA	1:B:646:MET:HG2	1.78	0.65
1:L:57:VAL:HG22	1:L:582:VAL:HG21	1.79	0.64
1:A:272:LEU:HD23	1:A:284:VAL:HG11	1.80	0.64
1:D:215:ARG:HG2	1:D:224:ILE:HG23	1.78	0.64
1:G:57:VAL:HG22	1:G:582:VAL:HG21	1.79	0.64
1:J:180:ASN:HA	1:J:567:GLU:HG3	1.79	0.64
1:B:347:LEU:HA	1:B:351:HIS:HB2	1.80	0.63
1:B:518:LYS:O	1:B:522:THR:OG1	2.17	0.63
1:E:282:LYS:HE2	1:E:405:ALA:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:LEU:HD21	1:G:366:ALA:HA	1.79	0.63
1:K:462:ARG:NH1	1:K:617:ASP:OD2	2.31	0.63
1:A:335:VAL:O	1:A:339:ASN:ND2	2.32	0.63
1:E:92:THR:HG23	1:E:147:VAL:HB	1.81	0.63
1:K:452:ASP:OD2	1:K:632:ARG:NH2	2.31	0.63
1:D:35:PRO:HB2	1:D:36:PRO:HD2	1.80	0.62
1:A:363:ARG:NH2	1:D:279:GLY:O	2.32	0.62
1:F:106:LEU:HD21	1:F:125:PRO:HG2	1.81	0.62
1:E:198:LEU:HD12	1:E:199:PRO:HD2	1.81	0.62
1:E:436:ARG:NH2	1:E:447:TYR:OH	2.32	0.62
1:F:34:LEU:HD23	1:F:37:LEU:HD12	1.81	0.62
1:L:95:GLU:HB2	1:L:147:VAL:HG21	1.79	0.62
1:E:242:LYS:HE3	1:E:247:GLU:HG3	1.80	0.62
1:I:212:ALA:HB2	1:I:302:PRO:HD3	1.82	0.62
1:G:110:GLU:HB3	1:G:595:PHE:CD1	2.35	0.62
1:D:111:ASN:O	1:D:113:ASP:N	2.33	0.61
1:K:198:LEU:HD12	1:K:199:PRO:HD2	1.81	0.61
1:H:109:LEU:HG	1:H:111:ASN:H	1.63	0.61
1:D:124:GLU:HB2	1:D:128:LEU:HB2	1.81	0.61
1:A:252:ASP:OD1	1:A:252:ASP:N	2.32	0.60
1:F:180:ASN:HA	1:F:567:GLU:HG3	1.83	0.60
1:K:95:GLU:HB2	1:K:147:VAL:HG21	1.82	0.60
1:G:198:LEU:HD12	1:G:199:PRO:HD2	1.83	0.60
1:E:279:GLY:O	1:G:363:ARG:NH2	2.34	0.60
1:F:373:MET:HA	1:F:600:TRP:HZ3	1.66	0.60
1:I:110:GLU:HB3	1:I:595:PHE:CE1	2.36	0.60
1:L:522:THR:HA	1:L:526:GLU:HB3	1.83	0.60
1:I:233:ASN:OD1	1:I:233:ASN:N	2.35	0.59
1:D:34:LEU:HD21	1:D:412:HIS:CE1	2.38	0.59
1:D:462:ARG:NH1	1:D:617:ASP:OD2	2.35	0.59
1:F:463:TRP:HZ3	1:F:610:LEU:HB3	1.68	0.59
1:G:373:MET:HA	1:G:600:TRP:HZ3	1.66	0.59
1:H:350:THR:OG1	1:H:351:HIS:N	2.35	0.59
1:J:174:VAL:HG11	1:J:567:GLU:HG2	1.84	0.59
1:F:522:THR:HA	1:F:526:GLU:HB3	1.83	0.59
1:J:585:THR:HG23	1:J:646:MET:H	1.68	0.59
1:G:596:PRO:HB2	1:G:598:ARG:HG3	1.84	0.59
1:A:214:TYR:OH	1:A:537:LEU:O	2.20	0.58
1:L:307:PRO:HB3	1:L:553:PRO:HG2	1.86	0.58
1:F:346:HIS:O	1:F:350:THR:OG1	2.16	0.58
1:B:346:HIS:O	1:B:350:THR:OG1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:508:THR:HG22	1:H:510:ALA:H	1.67	0.57
1:H:418:ALA:HA	1:H:421:ARG:HG2	1.85	0.57
1:I:552:ALA:HB1	1:I:554:PRO:HD2	1.86	0.57
1:I:587:LEU:HA	1:I:646:MET:HG2	1.85	0.57
1:J:346:HIS:O	1:J:350:THR:OG1	2.21	0.57
1:K:30:TYR:CE1	1:K:38:ALA:HB1	2.40	0.57
1:L:35:PRO:HB2	1:L:36:PRO:HD2	1.86	0.57
1:A:606:ILE:HA	1:A:610:LEU:HB2	1.85	0.57
1:L:260:LEU:HD22	1:L:290:LEU:HD11	1.85	0.57
1:A:109:LEU:O	1:A:111:ASN:N	2.38	0.57
1:L:215:ARG:N	1:L:215:ARG:HD2	2.20	0.57
1:C:96:ASP:OD1	1:C:134:ARG:NH2	2.36	0.56
1:B:455:LYS:HD3	1:B:624:LEU:HD23	1.86	0.56
1:A:243:GLN:HB3	1:A:321:GLN:HG2	1.87	0.56
1:G:580:GLY:O	3:G:801:HOH:O	2.18	0.56
1:B:552:ALA:HB1	1:B:554:PRO:HD2	1.87	0.56
1:G:231:PRO:HG2	1:G:234:PHE:HB3	1.86	0.56
1:C:215:ARG:N	1:C:215:ARG:HD2	2.21	0.56
1:C:408:ILE:O	1:C:412:HIS:ND1	2.38	0.56
1:F:64:VAL:HG13	1:F:574:GLU:HB3	1.88	0.56
1:F:198:LEU:HD12	1:F:199:PRO:HD2	1.87	0.56
1:G:180:ASN:HA	1:G:567:GLU:HG2	1.88	0.56
1:A:215:ARG:NH2	1:A:334:GLN:OE1	2.39	0.56
1:F:260:LEU:HD22	1:F:290:LEU:HD11	1.87	0.55
1:J:230:LEU:HD11	1:J:236:VAL:HG22	1.87	0.55
1:L:145:ARG:NH1	1:L:574:GLU:OE1	2.39	0.55
1:L:463:TRP:HZ3	1:L:610:LEU:HB3	1.70	0.55
1:G:433:ILE:HG23	1:G:438:VAL:HG23	1.89	0.55
1:K:522:THR:HG22	1:K:526:GLU:HG2	1.88	0.55
1:I:559:LEU:HG	1:I:563:GLN:HE21	1.70	0.55
1:J:403:ILE:HD11	1:J:571:LEU:HG	1.88	0.55
1:B:378:HIS:HD2	1:B:520:ILE:HG12	1.71	0.55
1:A:260:LEU:HD22	1:A:290:LEU:HD11	1.88	0.55
1:L:508:THR:HG22	1:L:510:ALA:H	1.72	0.55
1:B:89:VAL:HA	1:B:92:THR:HG22	1.87	0.55
1:J:57:VAL:HG22	1:J:650:ILE:HD11	1.89	0.55
1:I:452:ASP:HB3	1:I:639:MET:HB2	1.89	0.55
1:A:341:HIS:HA	1:A:345:SER:HB2	1.89	0.54
1:E:341:HIS:HA	1:E:345:SER:HB2	1.89	0.54
1:H:187:ASP:O	1:H:191:ASN:ND2	2.41	0.54
1:J:358:VAL:HG22	1:J:379:PHE:CG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:584:HIS:O	1:G:585:THR:HG22	2.07	0.54
1:H:436:ARG:NH2	1:H:447:TYR:OH	2.39	0.54
1:J:198:LEU:HD12	1:J:199:PRO:HD2	1.88	0.54
1:B:220:ASN:ND2	1:B:223:MET:HG3	2.21	0.54
1:G:341:HIS:HA	1:G:345:SER:HB2	1.88	0.54
1:J:92:THR:OG1	1:J:147:VAL:HB	2.08	0.54
1:K:230:LEU:HD11	1:K:251:LEU:HD21	1.90	0.54
1:L:214:TYR:HB3	1:L:215:ARG:NH1	2.22	0.54
1:D:373:MET:HA	1:D:600:TRP:CZ3	2.43	0.54
1:E:462:ARG:NH1	1:E:617:ASP:OD2	2.40	0.54
1:J:373:MET:HA	1:J:600:TRP:CZ3	2.43	0.54
1:K:39:PHE:HD1	1:K:40:CYS:H	1.56	0.54
1:B:629:ASN:HD21	1:B:635:LYS:HB3	1.73	0.54
1:B:234:PHE:HD2	1:B:262:LEU:HD11	1.72	0.54
1:B:622:GLU:HB2	1:B:641:PRO:HD2	1.89	0.54
1:C:268:ILE:HD11	1:C:340:TYR:HB2	1.89	0.54
1:C:584:HIS:O	1:C:585:THR:HG22	2.08	0.54
1:E:35:PRO:O	1:E:37:LEU:N	2.35	0.54
1:K:231:PRO:HG2	1:K:234:PHE:HB3	1.89	0.54
1:G:524:SER:OG	1:G:525:ALA:N	2.39	0.54
1:J:584:HIS:O	1:J:585:THR:HG22	2.07	0.54
1:C:462:ARG:NH1	1:C:617:ASP:OD2	2.41	0.53
1:D:95:GLU:HB2	1:D:147:VAL:HG21	1.90	0.53
1:D:373:MET:HA	1:D:600:TRP:HZ3	1.72	0.53
1:A:527:HIS:CG	1:A:648:ILE:HG12	2.42	0.53
1:B:231:PRO:HG2	1:B:234:PHE:HB3	1.90	0.53
1:D:585:THR:CG2	1:D:646:MET:H	2.17	0.53
1:F:272:LEU:HD11	1:F:414:LEU:HD22	1.90	0.53
1:H:452:ASP:HB3	1:H:639:MET:HB2	1.90	0.53
1:I:584:HIS:O	1:I:585:THR:HG22	2.08	0.53
1:E:35:PRO:HB2	1:E:36:PRO:HD2	1.90	0.53
1:H:198:LEU:HD12	1:H:199:PRO:HD2	1.90	0.53
1:J:462:ARG:NH1	1:J:617:ASP:OD2	2.41	0.53
1:F:215:ARG:HD2	1:F:215:ARG:N	2.24	0.53
1:G:240:HIS:CD2	1:G:319:ALA:HB2	2.44	0.53
1:G:373:MET:HA	1:G:600:TRP:CZ3	2.42	0.53
1:I:147:VAL:HB	1:I:150:ALA:HB3	1.90	0.53
1:I:268:ILE:HG23	1:I:272:LEU:HD22	1.91	0.53
1:L:385:ILE:HG12	1:L:650:ILE:HA	1.90	0.53
1:A:110:GLU:HB3	1:A:595:PHE:CE1	2.44	0.53
1:D:198:LEU:HD12	1:D:199:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:TYR:HB3	1:G:215:ARG:NH1	2.24	0.53
1:J:6:THR:OG1	1:J:11:ASP:OD1	2.27	0.53
1:A:25:ARG:HG2	1:A:363:ARG:HB3	1.90	0.53
1:B:215:ARG:HD2	1:B:215:ARG:N	2.24	0.53
1:C:268:ILE:HG23	1:C:272:LEU:HD22	1.91	0.53
1:I:308:GLY:N	1:I:315:ASN:OD1	2.37	0.53
1:A:35:PRO:HB2	1:A:36:PRO:HD2	1.91	0.52
1:H:187:ASP:OD1	1:H:187:ASP:N	2.42	0.52
1:E:606:ILE:HA	1:E:610:LEU:HB2	1.91	0.52
1:H:358:VAL:HG22	1:H:379:PHE:CG	2.44	0.52
1:J:268:ILE:HG23	1:J:272:LEU:HD13	1.89	0.52
1:L:272:LEU:HA	1:L:410:SER:HB2	1.91	0.52
1:C:637:THR:HA	1:C:640:ILE:HD13	1.90	0.52
1:J:89:VAL:HA	1:J:92:THR:HG22	1.90	0.52
1:J:187:ASP:N	1:J:187:ASP:OD1	2.42	0.52
1:L:318:TYR:OH	1:L:554:PRO:HD3	2.10	0.52
1:C:57:VAL:HG22	1:C:582:VAL:HG21	1.91	0.52
1:F:584:HIS:O	1:F:585:THR:HG22	2.10	0.52
1:I:606:ILE:HA	1:I:610:LEU:HB2	1.92	0.52
1:J:109:LEU:O	1:J:111:ASN:N	2.41	0.52
1:K:318:TYR:OH	1:K:554:PRO:HD3	2.10	0.52
1:B:378:HIS:CD2	1:B:520:ILE:HG12	2.43	0.52
1:H:272:LEU:HD23	1:H:284:VAL:HG11	1.92	0.52
1:C:211:PHE:CG	1:C:330:LYS:HD2	2.44	0.51
1:G:527:HIS:CG	1:G:648:ILE:HG12	2.43	0.51
1:J:318:TYR:OH	1:J:554:PRO:HD3	2.09	0.51
1:K:433:ILE:HG23	1:K:438:VAL:HG23	1.92	0.51
1:A:318:TYR:OH	1:A:554:PRO:HD3	2.11	0.51
1:B:174:VAL:HG22	1:B:175:SER:H	1.75	0.51
1:G:260:LEU:HD22	1:G:290:LEU:HD11	1.93	0.51
1:H:373:MET:HA	1:H:600:TRP:HZ3	1.74	0.51
1:A:215:ARG:HD2	1:A:215:ARG:N	2.25	0.51
1:F:307:PRO:HB3	1:F:553:PRO:HG2	1.91	0.51
1:H:139:LEU:HD22	1:H:393:LEU:HD13	1.92	0.51
1:L:373:MET:HA	1:L:600:TRP:HZ3	1.75	0.51
1:B:53:TRP:HE1	1:B:649:ASN:HB2	1.75	0.51
1:H:241:TYR:CZ	1:H:245:MET:HG3	2.46	0.51
1:H:584:HIS:O	1:H:585:THR:HG22	2.10	0.51
1:B:265:TRP:HB2	1:B:287:PRO:HD2	1.91	0.51
1:B:522:THR:HA	1:B:526:GLU:HB3	1.93	0.51
1:H:180:ASN:HA	1:H:567:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:255:LYS:HB3	1:K:260:LEU:HD12	1.93	0.51
1:K:316:LYS:HB3	1:K:316:LYS:HZ2	1.76	0.51
1:C:214:TYR:HB3	1:C:215:ARG:NH1	2.25	0.51
1:D:231:PRO:HG2	1:D:234:PHE:HB3	1.91	0.51
1:C:282:LYS:HB3	1:C:547:ALA:HB1	1.93	0.51
1:E:460:ILE:HD13	1:E:520:ILE:HG22	1.92	0.51
1:E:471:TYR:HE2	1:E:606:ILE:HD11	1.76	0.51
1:E:649:ASN:ND2	3:E:801:HOH:O	2.44	0.51
1:F:135:VAL:HG22	1:F:578:LEU:HD21	1.92	0.51
1:I:272:LEU:HD11	1:I:414:LEU:HD22	1.93	0.51
1:K:215:ARG:HD2	1:K:215:ARG:N	2.25	0.51
1:L:147:VAL:HB	1:L:150:ALA:HB2	1.92	0.51
1:C:182:ARG:HE	1:C:183:PRO:HD2	1.75	0.51
1:C:272:LEU:HA	1:C:410:SER:HB2	1.93	0.51
1:A:231:PRO:HG2	1:A:234:PHE:HB3	1.93	0.50
1:E:182:ARG:HH21	1:E:561:ASP:HA	1.76	0.50
1:F:264:ASP:OD1	1:F:265:TRP:N	2.44	0.50
1:K:145:ARG:NH1	3:K:801:HOH:O	2.43	0.50
1:C:622:GLU:HB2	1:C:641:PRO:HD2	1.93	0.50
1:K:307:PRO:HB3	1:K:553:PRO:HG2	1.93	0.50
1:D:260:LEU:HD22	1:D:290:LEU:HD11	1.93	0.50
1:H:373:MET:HA	1:H:600:TRP:CZ3	2.46	0.50
1:J:134:ARG:HH21	1:J:148:PRO:HG3	1.77	0.50
1:D:573:ALA:O	1:D:577:TYR:HB2	2.11	0.50
1:H:215:ARG:HD2	1:H:215:ARG:N	2.26	0.50
1:J:552:ALA:HB1	1:J:554:PRO:HD2	1.92	0.50
1:A:522:THR:HG22	1:A:526:GLU:HG2	1.93	0.50
1:A:373:MET:HA	1:A:600:TRP:CH2	2.47	0.50
1:J:64:VAL:HG13	1:J:574:GLU:HB3	1.94	0.50
1:J:134:ARG:NH2	1:J:148:PRO:HG3	2.27	0.50
1:E:215:ARG:N	1:E:215:ARG:HD2	2.27	0.50
1:G:35:PRO:HB3	1:G:36:PRO:HD2	1.93	0.50
1:A:139:LEU:HD22	1:A:393:LEU:HD13	1.94	0.49
1:F:30:TYR:CE1	1:F:38:ALA:HB1	2.46	0.49
1:I:436:ARG:NH2	1:I:447:TYR:OH	2.45	0.49
1:F:54:LEU:HD13	1:F:127:VAL:HB	1.94	0.49
1:A:460:ILE:HD13	1:A:520:ILE:HG22	1.95	0.49
1:L:198:LEU:HD12	1:L:199:PRO:HD2	1.93	0.49
1:A:241:TYR:CZ	1:A:245:MET:HG3	2.47	0.49
1:C:277:TYR:OH	1:C:567:GLU:OE1	2.18	0.49
1:D:106:LEU:HD22	1:D:126:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:463:TRP:HB2	1:G:614:PHE:HB2	1.94	0.49
1:H:34:LEU:HD11	1:H:412:HIS:CE1	2.47	0.49
1:J:471:TYR:HE2	1:J:606:ILE:HD11	1.77	0.49
1:G:403:ILE:HG21	1:G:572:GLN:HB2	1.94	0.49
1:I:215:ARG:HD2	1:I:215:ARG:N	2.28	0.49
1:L:275:ASN:HB2	1:L:407:THR:HG22	1.94	0.49
1:A:268:ILE:HG23	1:A:272:LEU:HD22	1.94	0.49
1:E:241:TYR:CZ	1:E:245:MET:HG3	2.48	0.49
1:E:316:LYS:NZ	1:E:317:ILE:H	2.10	0.49
1:B:92:THR:OG1	1:B:147:VAL:HB	2.13	0.49
1:L:358:VAL:HG22	1:L:379:PHE:CG	2.47	0.49
1:G:471:TYR:OH	1:G:606:ILE:HD11	2.13	0.49
1:I:265:TRP:HB2	1:I:287:PRO:HD2	1.95	0.49
1:K:377:PRO:HD3	1:K:600:TRP:CZ3	2.47	0.49
1:C:351:HIS:ND1	1:C:386:ASN:OD1	2.42	0.49
1:G:92:THR:HG23	1:G:147:VAL:HB	1.95	0.49
1:D:109:LEU:O	1:D:111:ASN:N	2.40	0.49
1:F:214:TYR:HB3	1:F:215:ARG:NH1	2.28	0.49
1:A:433:ILE:HG23	1:A:438:VAL:HG23	1.93	0.48
1:D:69:VAL:HG11	1:D:93:SER:HB2	1.93	0.48
1:J:294:PRO:HG2	1:J:298:GLY:HA3	1.94	0.48
1:B:214:TYR:HB3	1:B:215:ARG:NH1	2.28	0.48
1:G:227:ILE:HD13	1:G:262:LEU:HB2	1.95	0.48
1:B:212:ALA:HB2	1:B:302:PRO:HD3	1.94	0.48
1:F:385:ILE:HG12	1:F:650:ILE:C	2.33	0.48
1:B:215:ARG:HD2	1:B:215:ARG:H	1.78	0.48
1:F:373:MET:HA	1:F:600:TRP:CZ3	2.47	0.48
1:I:94:GLU:O	1:I:98:ASN:N	2.45	0.48
1:H:174:VAL:HG11	1:H:567:GLU:HB3	1.94	0.48
1:K:372:TYR:CZ	1:K:376:ILE:HG13	2.48	0.48
1:E:584:HIS:O	1:E:585:THR:HG22	2.13	0.48
1:B:372:TYR:CZ	1:B:376:ILE:HG13	2.49	0.48
1:I:486:ALA:O	1:I:490:VAL:HG12	2.13	0.48
1:J:60:VAL:HG12	1:J:578:LEU:HD12	1.94	0.48
1:D:11:ASP:OD2	1:D:17:ARG:NH1	2.43	0.48
1:D:346:HIS:O	1:D:350:THR:OG1	2.22	0.48
1:H:377:PRO:HD3	1:H:600:TRP:CZ3	2.49	0.48
1:I:373:MET:HA	1:I:600:TRP:CZ3	2.49	0.48
1:J:436:ARG:NH2	1:J:447:TYR:OH	2.47	0.48
1:A:534:GLN:HA	1:A:538:MET:HE2	1.96	0.48
1:B:234:PHE:CD2	1:B:262:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:ARG:HH22	1:G:561:ASP:HA	1.79	0.48
1:I:373:MET:HA	1:I:600:TRP:HZ3	1.79	0.48
1:D:606:ILE:HA	1:D:610:LEU:HB2	1.95	0.48
1:J:629:ASN:OD1	1:J:636:TYR:N	2.47	0.48
1:B:225:GLN:HG3	1:B:436:ARG:HA	1.95	0.47
1:B:533:PRO:HG3	1:B:638:TYR:CE2	2.49	0.47
1:D:605:LYS:O	1:D:609:GLU:HB3	2.13	0.47
1:L:231:PRO:HG2	1:L:234:PHE:HB3	1.96	0.47
1:C:593:ASN:N	1:C:593:ASN:OD1	2.47	0.47
1:D:584:HIS:O	1:D:585:THR:HG22	2.13	0.47
1:E:433:ILE:HG23	1:E:438:VAL:HG23	1.96	0.47
1:E:463:TRP:HZ3	1:E:610:LEU:HB3	1.79	0.47
1:G:144:ASN:O	1:G:144:ASN:ND2	2.47	0.47
1:L:211:PHE:CG	1:L:330:LYS:HD2	2.49	0.47
1:L:389:ALA:O	1:L:394:ILE:HG12	2.14	0.47
1:L:456:ILE:HD11	1:L:641:PRO:HG3	1.96	0.47
1:L:585:THR:O	1:L:645:PRO:HA	2.14	0.47
1:D:528:SER:HB2	1:D:645:PRO:HD2	1.96	0.47
1:G:174:VAL:HG23	1:G:278:LYS:NZ	2.29	0.47
1:K:211:PHE:CG	1:K:330:LYS:HD2	2.50	0.47
1:D:553:PRO:O	1:D:555:SER:N	2.48	0.47
1:B:255:LYS:HB3	1:B:260:LEU:HD12	1.96	0.47
1:B:603:ASP:O	1:B:607:THR:OG1	2.32	0.47
1:D:64:VAL:HG13	1:D:574:GLU:HB3	1.96	0.47
1:G:586:LYS:HA	1:G:586:LYS:HD3	1.73	0.47
1:B:355:GLU:OE1	1:B:386:ASN:ND2	2.38	0.47
1:F:358:VAL:HG22	1:F:379:PHE:CG	2.50	0.47
1:G:558:PRO:HB2	1:G:560:LYS:HG3	1.96	0.47
1:J:227:ILE:HD13	1:J:262:LEU:HB2	1.97	0.47
1:K:584:HIS:O	1:K:585:THR:HG22	2.14	0.47
1:A:373:MET:HA	1:A:600:TRP:HH2	1.78	0.47
1:A:429:LEU:HD22	1:A:521:PHE:CZ	2.49	0.47
1:E:373:MET:HA	1:E:600:TRP:HZ3	1.79	0.47
1:H:452:ASP:OD2	1:H:632:ARG:NH2	2.48	0.47
1:L:268:ILE:HG23	1:L:272:LEU:HD22	1.97	0.47
1:A:347:LEU:HA	1:A:351:HIS:HB2	1.97	0.47
1:C:92:THR:HG23	1:C:147:VAL:HG22	1.96	0.47
1:H:231:PRO:HG2	1:H:234:PHE:HB3	1.97	0.47
1:A:377:PRO:HD3	1:A:600:TRP:CH2	2.49	0.47
1:C:358:VAL:HG22	1:C:379:PHE:CG	2.50	0.47
1:G:473:ILE:H	1:G:477:ASN:HD22	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:522:THR:HG22	1:H:526:GLU:HG2	1.97	0.47
1:I:268:ILE:HD11	1:I:340:TYR:HB2	1.97	0.47
1:J:110:GLU:HB3	1:J:595:PHE:HE1	1.79	0.47
1:C:533:PRO:HG3	1:C:638:TYR:CE2	2.50	0.46
1:G:377:PRO:HD3	1:G:600:TRP:CZ3	2.50	0.46
1:H:265:TRP:HB2	1:H:287:PRO:HD2	1.96	0.46
1:J:460:ILE:HD13	1:J:520:ILE:HG22	1.97	0.46
1:J:524:SER:OG	1:J:525:ALA:N	2.47	0.46
1:K:139:LEU:HD22	1:K:393:LEU:HD13	1.97	0.46
1:K:307:PRO:HG2	1:K:315:ASN:ND2	2.30	0.46
1:A:35:PRO:O	1:A:37:LEU:N	2.42	0.46
1:A:358:VAL:HG22	1:A:379:PHE:CG	2.50	0.46
1:F:318:TYR:OH	1:F:554:PRO:HD3	2.15	0.46
1:A:341:HIS:O	1:A:346:HIS:N	2.46	0.46
1:A:629:ASN:HD21	1:A:636:TYR:H	1.63	0.46
1:D:460:ILE:HD13	1:D:520:ILE:HG22	1.98	0.46
1:F:189:TYR:OH	1:F:563:GLN:HB2	2.14	0.46
1:F:211:PHE:CG	1:F:330:LYS:HD2	2.51	0.46
1:H:308:GLY:N	1:H:315:ASN:HD21	2.13	0.46
1:J:553:PRO:N	1:J:554:PRO:HD2	2.30	0.46
1:L:534:GLN:HB3	1:L:576:LEU:HD22	1.96	0.46
1:A:51:ALA:HA	1:A:54:LEU:HD12	1.97	0.46
1:K:205:TRP:CZ2	1:K:206:LYS:HE2	2.50	0.46
1:L:216:VAL:HB	1:L:447:TYR:HA	1.96	0.46
1:I:53:TRP:HE3	1:I:54:LEU:HD23	1.80	0.46
1:I:573:ALA:O	1:I:577:TYR:HB2	2.15	0.46
1:L:92:THR:OG1	1:L:146:HIS:HB3	2.15	0.46
1:A:508:THR:HG22	1:A:510:ALA:H	1.80	0.46
1:B:603:ASP:HB3	1:B:606:ILE:HD12	1.98	0.46
1:H:277:TYR:OH	1:H:567:GLU:OE1	2.12	0.46
1:K:508:THR:HG22	1:K:510:ALA:H	1.81	0.46
1:B:183:PRO:HB3	1:B:566:LEU:HD21	1.98	0.46
1:C:373:MET:HA	1:C:600:TRP:HZ3	1.79	0.46
1:C:408:ILE:HG13	1:C:412:HIS:CE1	2.51	0.46
1:D:49:PRO:HB3	1:D:53:TRP:CE3	2.51	0.46
1:H:30:TYR:HE1	1:H:38:ALA:HB1	1.81	0.46
1:L:341:HIS:HA	1:L:345:SER:HB2	1.98	0.46
1:A:452:ASP:HB3	1:A:639:MET:HB2	1.98	0.46
1:B:260:LEU:HD22	1:B:290:LEU:HD11	1.98	0.46
1:C:198:LEU:HD12	1:C:199:PRO:HD2	1.98	0.46
1:C:460:ILE:HD13	1:C:520:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:ASN:HB2	1:H:309:GLN:O	2.16	0.46
1:K:53:TRP:CZ2	1:K:57:VAL:HG21	2.50	0.46
1:A:180:ASN:HA	1:A:567:GLU:HG3	1.98	0.46
1:I:403:ILE:HD11	1:I:571:LEU:HG	1.98	0.46
1:B:20:GLN:NE2	1:B:367:GLN:HG3	2.31	0.46
1:B:504:GLY:HA2	1:B:505:PRO:HA	1.67	0.46
1:H:205:TRP:CZ2	1:H:206:LYS:HE2	2.51	0.46
1:E:358:VAL:HG22	1:E:379:PHE:CG	2.51	0.45
1:E:637:THR:HG22	1:E:640:ILE:HD12	1.97	0.45
1:F:403:ILE:HA	1:F:568:LEU:HD13	1.98	0.45
1:G:30:TYR:CE1	1:G:38:ALA:HB1	2.51	0.45
1:B:224:ILE:HG13	1:B:438:VAL:HG11	1.98	0.45
1:H:334:GLN:HE21	1:H:544:ILE:HB	1.80	0.45
1:J:191:ASN:O	1:J:194:ARG:HG3	2.16	0.45
1:B:307:PRO:HG3	1:B:553:PRO:HG2	1.98	0.45
1:B:372:TYR:CE2	1:B:376:ILE:HG13	2.51	0.45
1:C:389:ALA:O	1:C:394:ILE:HG12	2.16	0.45
1:D:533:PRO:HG3	1:D:638:TYR:CE2	2.52	0.45
1:G:637:THR:HG22	1:G:640:ILE:HD12	1.96	0.45
1:I:183:PRO:HG2	1:I:560:LYS:HB2	1.98	0.45
1:G:35:PRO:CB	1:G:36:PRO:HD2	2.45	0.45
1:G:378:HIS:CE1	1:G:520:ILE:HG23	2.52	0.45
1:J:606:ILE:HA	1:J:610:LEU:HB2	1.99	0.45
1:D:452:ASP:HB3	1:D:639:MET:HB2	1.97	0.45
1:I:214:TYR:HB3	1:I:215:ARG:NH1	2.31	0.45
1:H:460:ILE:HD12	1:H:521:PHE:HD1	1.82	0.45
1:H:585:THR:O	1:H:645:PRO:HA	2.16	0.45
1:K:260:LEU:HD22	1:K:290:LEU:HD11	1.98	0.45
1:B:358:VAL:HG22	1:B:379:PHE:CG	2.52	0.45
1:D:377:PRO:HD3	1:D:600:TRP:CZ3	2.51	0.45
1:E:215:ARG:HD2	1:E:215:ARG:H	1.80	0.45
1:J:215:ARG:N	1:J:215:ARG:HD2	2.31	0.45
1:K:460:ILE:HD13	1:K:520:ILE:HG22	1.98	0.45
1:L:346:HIS:HD2	1:L:530:VAL:HG23	1.82	0.45
1:L:583:HIS:HB3	1:L:586:LYS:NZ	2.32	0.45
1:H:471:TYR:OH	1:H:606:ILE:HD11	2.17	0.45
1:A:56:THR:HG22	1:A:582:VAL:HG13	1.99	0.45
1:A:451:ASP:O	1:A:455:LYS:HG3	2.17	0.45
1:B:606:ILE:HA	1:B:610:LEU:HB2	1.99	0.45
1:C:35:PRO:CB	1:C:36:PRO:HD2	2.47	0.45
1:C:606:ILE:HA	1:C:610:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:VAL:HG22	1:I:175:SER:H	1.82	0.45
1:J:35:PRO:HB3	1:J:36:PRO:HD2	1.99	0.45
1:C:590:TYR:CE2	1:C:646:MET:HE1	2.52	0.45
1:D:460:ILE:HG22	1:D:517:THR:HG23	1.98	0.45
1:E:553:PRO:O	1:E:555:SER:N	2.50	0.45
1:I:30:TYR:CE1	1:I:38:ALA:HB1	2.52	0.45
1:L:463:TRP:HB2	1:L:614:PHE:HB2	1.97	0.45
1:A:429:LEU:O	1:A:433:ILE:HG12	2.17	0.44
1:A:582:VAL:HB	1:A:650:ILE:HD12	1.99	0.44
1:D:429:LEU:O	1:D:433:ILE:HG12	2.17	0.44
1:E:330:LYS:HB2	1:E:330:LYS:HE3	1.83	0.44
1:F:264:ASP:OD1	1:F:266:LYS:N	2.51	0.44
1:K:131:VAL:O	1:K:135:VAL:HG23	2.18	0.44
1:L:180:ASN:HA	1:L:567:GLU:HG3	2.00	0.44
1:C:215:ARG:HD2	1:C:215:ARG:H	1.81	0.44
1:C:329:ALA:HA	1:C:553:PRO:HB3	1.99	0.44
1:E:188:ASP:O	1:E:192:LEU:HG	2.17	0.44
1:G:358:VAL:HG22	1:G:379:PHE:CG	2.52	0.44
1:J:307:PRO:HG2	1:J:315:ASN:ND2	2.33	0.44
1:J:377:PRO:HD3	1:J:600:TRP:CZ3	2.52	0.44
1:B:30:TYR:CE1	1:B:38:ALA:HB1	2.52	0.44
1:G:225:GLN:HG3	1:G:436:ARG:HA	2.00	0.44
1:J:573:ALA:O	1:J:577:TYR:HB2	2.18	0.44
1:L:377:PRO:HD3	1:L:600:TRP:CZ3	2.52	0.44
1:B:373:MET:O	1:B:600:TRP:HZ3	2.01	0.44
1:C:276:THR:HG22	1:C:281:GLN:HA	2.00	0.44
1:F:606:ILE:HA	1:F:610:LEU:HB2	1.99	0.44
1:G:287:PRO:HG2	1:G:333:VAL:HA	2.00	0.44
1:I:376:ILE:HD13	1:I:379:PHE:HD2	1.81	0.44
1:I:463:TRP:HB2	1:I:614:PHE:CD1	2.52	0.44
1:I:377:PRO:HD3	1:I:600:TRP:CZ3	2.53	0.44
1:K:334:GLN:HE21	1:K:544:ILE:HB	1.82	0.44
1:K:552:ALA:HB1	1:K:554:PRO:HD2	1.98	0.44
1:E:11:ASP:OD2	1:E:17:ARG:NH1	2.48	0.44
1:G:372:TYR:CZ	1:G:376:ILE:HG13	2.53	0.44
1:J:110:GLU:HB3	1:J:595:PHE:CE1	2.52	0.44
1:J:214:TYR:HB3	1:J:215:ARG:NH1	2.33	0.44
1:A:594:SER:HB3	1:A:596:PRO:HD2	1.98	0.44
1:B:640:ILE:O	1:B:644:ILE:HG13	2.18	0.44
1:D:291:PHE:HB3	1:D:300:LEU:HG	2.00	0.44
1:H:147:VAL:HG12	1:H:148:PRO:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:450:ARG:NE	1:H:451:ASP:OD1	2.48	0.44
1:I:230:LEU:HD13	1:I:236:VAL:HG13	1.99	0.44
1:L:34:LEU:HD11	1:L:412:HIS:CE1	2.53	0.44
1:E:573:ALA:O	1:E:577:TYR:HB2	2.18	0.44
1:G:622:GLU:HB2	1:G:641:PRO:HD2	2.00	0.44
1:H:214:TYR:HB3	1:H:215:ARG:NH1	2.33	0.44
1:I:240:HIS:CD2	1:I:319:ALA:HB2	2.47	0.44
1:I:409:GLU:O	1:I:413:GLN:HG2	2.18	0.44
1:L:95:GLU:HB3	1:L:147:VAL:HG11	2.00	0.44
1:A:265:TRP:HB2	1:A:287:PRO:HD2	2.00	0.43
1:D:142:LYS:HA	1:D:142:LYS:HD3	1.64	0.43
1:G:215:ARG:HD2	1:G:215:ARG:N	2.32	0.43
1:I:233:ASN:O	1:I:311:PRO:HG3	2.19	0.43
1:K:567:GLU:H	1:K:567:GLU:HG3	1.38	0.43
1:L:144:ASN:O	1:L:144:ASN:ND2	2.52	0.43
1:L:265:TRP:HB2	1:L:287:PRO:HD2	1.99	0.43
1:A:92:THR:HG21	1:A:146:HIS:HB3	1.99	0.43
1:D:545:THR:OG1	1:D:546:GLY:N	2.50	0.43
1:E:534:GLN:HA	1:E:538:MET:HB2	2.01	0.43
1:F:409:GLU:O	1:F:413:GLN:HG2	2.18	0.43
1:H:533:PRO:HG3	1:H:638:TYR:CE2	2.53	0.43
1:I:21:LEU:HD23	1:I:21:LEU:HA	1.80	0.43
1:I:106:LEU:HD22	1:I:126:SER:HB3	1.99	0.43
1:L:102:HIS:O	1:L:106:LEU:HB2	2.17	0.43
1:E:174:VAL:HG21	1:E:567:GLU:HB3	1.99	0.43
1:G:173:ASN:HD22	1:L:29:LYS:NZ	2.16	0.43
1:B:531:ASN:ND2	1:B:534:GLN:OE1	2.52	0.43
1:C:527:HIS:NE2	1:C:648:ILE:HG23	2.33	0.43
1:G:212:ALA:HB2	1:G:302:PRO:HD3	2.00	0.43
1:J:635:LYS:HE3	1:J:635:LYS:HB3	1.87	0.43
1:B:216:VAL:HG13	1:B:300:LEU:HD22	2.01	0.43
1:I:231:PRO:HG2	1:I:234:PHE:HB3	2.01	0.43
1:J:316:LYS:HE2	1:J:316:LYS:HA	2.00	0.43
1:K:358:VAL:HG22	1:K:379:PHE:CG	2.54	0.43
1:K:429:LEU:O	1:K:433:ILE:HG12	2.18	0.43
1:A:53:TRP:CE3	1:A:54:LEU:HD23	2.53	0.43
1:A:230:LEU:HD11	1:A:236:VAL:HG22	2.01	0.43
1:A:282:LYS:HB3	1:A:547:ALA:HB1	2.01	0.43
1:B:134:ARG:CZ	1:B:148:PRO:HG2	2.49	0.43
1:C:373:MET:HA	1:C:600:TRP:CZ3	2.53	0.43
1:H:559:LEU:O	1:H:563:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:463:TRP:HB2	1:J:614:PHE:CD1	2.53	0.43
1:J:527:HIS:CG	1:J:648:ILE:HG12	2.54	0.43
1:K:201:ILE:HG12	1:K:214:TYR:OH	2.18	0.43
1:L:35:PRO:CB	1:L:36:PRO:HD2	2.47	0.43
1:L:372:TYR:CE2	1:L:376:ILE:HG13	2.54	0.43
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.82	0.43
1:C:408:ILE:HG13	1:C:412:HIS:HE1	1.84	0.43
1:E:57:VAL:HG22	1:E:582:VAL:HG21	1.99	0.43
1:G:533:PRO:HG3	1:G:638:TYR:CE2	2.54	0.43
1:I:211:PHE:CG	1:I:330:LYS:HD2	2.53	0.43
1:I:585:THR:O	1:I:645:PRO:HA	2.18	0.43
1:L:174:VAL:HG11	1:L:567:GLU:HB3	2.01	0.43
1:C:102:HIS:O	1:C:106:LEU:HB2	2.19	0.43
1:C:612:PRO:O	1:C:616:ARG:HG3	2.19	0.43
1:D:145:ARG:H	1:D:145:ARG:HG3	1.41	0.43
1:D:358:VAL:HG22	1:D:379:PHE:CG	2.54	0.43
1:F:215:ARG:HD2	1:F:215:ARG:H	1.84	0.43
1:G:139:LEU:HD22	1:G:393:LEU:HD13	2.00	0.43
1:L:373:MET:HA	1:L:600:TRP:CZ3	2.54	0.43
1:A:35:PRO:C	1:A:37:LEU:H	2.21	0.43
1:B:69:VAL:HG11	1:B:93:SER:HB2	2.00	0.43
1:F:20:GLN:NE2	1:F:367:GLN:HG3	2.34	0.43
1:F:585:THR:O	1:F:645:PRO:HA	2.19	0.43
1:G:233:ASN:O	1:G:306:GLN:NE2	2.45	0.43
1:G:316:LYS:NZ	1:G:317:ILE:H	2.17	0.43
1:H:462:ARG:NH1	1:H:617:ASP:OD2	2.47	0.43
1:I:504:GLY:HA2	1:I:505:PRO:HA	1.70	0.43
1:J:341:HIS:O	1:J:346:HIS:N	2.50	0.43
1:A:35:PRO:CB	1:A:36:PRO:HD2	2.49	0.42
1:A:307:PRO:HB3	1:A:553:PRO:HG2	2.01	0.42
1:B:125:PRO:HB2	1:B:126:SER:H	1.52	0.42
1:B:408:ILE:HD12	1:B:408:ILE:HA	1.91	0.42
1:C:37:LEU:HD23	1:C:37:LEU:HA	1.87	0.42
1:I:37:LEU:HD23	1:I:37:LEU:HA	1.82	0.42
1:J:408:ILE:HD12	1:J:408:ILE:HA	1.85	0.42
1:C:65:ALA:O	1:C:69:VAL:HG23	2.19	0.42
1:D:203:SER:O	1:K:10:ASN:HB3	2.19	0.42
1:E:429:LEU:O	1:E:433:ILE:HG12	2.19	0.42
1:G:76:LYS:HB3	1:G:76:LYS:HE2	1.78	0.42
1:J:87:PHE:O	1:J:91:GLY:N	2.45	0.42
1:L:553:PRO:N	1:L:554:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:612:PRO:O	1:L:616:ARG:HG3	2.19	0.42
1:C:538:MET:HG2	1:C:544:ILE:HD13	2.01	0.42
1:F:533:PRO:HG3	1:F:638:TYR:CE2	2.54	0.42
1:F:586:LYS:HA	1:F:586:LYS:HD3	1.74	0.42
1:G:606:ILE:HA	1:G:610:LEU:HB2	2.00	0.42
1:H:610:LEU:HA	1:H:610:LEU:HD12	1.73	0.42
1:K:125:PRO:HB2	1:K:126:SER:H	1.63	0.42
1:A:553:PRO:N	1:A:554:PRO:HD2	2.34	0.42
1:B:147:VAL:HG22	1:B:148:PRO:O	2.20	0.42
1:C:377:PRO:HD3	1:C:600:TRP:CZ3	2.54	0.42
1:D:582:VAL:HB	1:D:650:ILE:HG13	2.02	0.42
1:F:33:LEU:HD12	1:F:39:PHE:CD1	2.54	0.42
1:F:35:PRO:CB	1:F:36:PRO:HD2	2.49	0.42
1:F:316:LYS:HD2	1:F:316:LYS:HA	1.66	0.42
1:G:467:TYR:HE2	1:G:606:ILE:HD13	1.84	0.42
1:H:30:TYR:CE1	1:H:38:ALA:HB1	2.53	0.42
1:D:376:ILE:HD13	1:D:376:ILE:HA	1.88	0.42
1:D:567:GLU:H	1:D:567:GLU:HG3	1.47	0.42
1:E:604:PRO:HA	1:E:607:THR:HB	2.02	0.42
1:F:307:PRO:HG2	1:F:315:ASN:ND2	2.35	0.42
1:K:174:VAL:HG11	1:K:567:GLU:HB3	2.01	0.42
1:K:353:LEU:O	1:K:356:PRO:HD2	2.19	0.42
1:L:422:HIS:O	1:L:501:SER:HB2	2.20	0.42
1:A:139:LEU:HD21	1:A:579:LEU:HD21	2.01	0.42
1:D:34:LEU:HA	1:D:34:LEU:HD22	1.68	0.42
1:G:376:ILE:N	1:G:377:PRO:HD2	2.35	0.42
1:J:635:LYS:H	1:J:635:LYS:HG2	1.53	0.42
1:K:53:TRP:CE2	1:K:57:VAL:HG21	2.54	0.42
1:B:284:VAL:HG23	1:B:335:VAL:HG12	2.02	0.42
1:C:87:PHE:HD1	1:C:87:PHE:HA	1.71	0.42
1:D:553:PRO:N	1:D:554:PRO:HD2	2.35	0.42
1:E:110:GLU:HB3	1:E:595:PHE:CD1	2.55	0.42
1:H:330:LYS:HE3	1:H:330:LYS:HB2	1.76	0.42
1:L:438:VAL:O	1:L:450:ARG:NH1	2.43	0.42
1:C:252:ASP:HA	1:C:255:LYS:HG2	2.01	0.42
1:C:573:ALA:O	1:C:577:TYR:HB2	2.20	0.42
1:E:51:ALA:O	1:E:55:VAL:HG23	2.20	0.42
1:E:307:PRO:HB3	1:E:553:PRO:HG2	2.01	0.42
1:H:192:LEU:HD22	1:H:570:GLU:HB2	2.02	0.42
1:K:20:GLN:NE2	1:K:367:GLN:HG3	2.35	0.42
1:C:30:TYR:CE1	1:C:38:ALA:HB1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:HIS:HA	1:D:345:SER:HB2	2.02	0.42
1:E:145:ARG:NH1	1:E:574:GLU:OE1	2.53	0.42
1:E:307:PRO:HG2	1:E:315:ASN:ND2	2.34	0.42
1:K:57:VAL:HG22	1:K:582:VAL:HG21	2.02	0.42
1:K:273:VAL:O	1:K:406:GLY:HA2	2.20	0.42
1:L:45:LYS:HA	1:L:45:LYS:HD2	1.87	0.42
1:L:606:ILE:HA	1:L:610:LEU:HB2	2.02	0.42
1:A:567:GLU:HG3	1:A:567:GLU:H	1.44	0.42
1:D:77:ARG:H	1:D:77:ARG:HG3	1.53	0.42
1:D:588:GLY:O	1:D:615:GLN:NE2	2.51	0.42
1:E:471:TYR:CE2	1:E:606:ILE:HD11	2.53	0.42
1:E:533:PRO:HG3	1:E:638:TYR:CE2	2.55	0.42
1:F:87:PHE:O	1:F:91:GLY:N	2.44	0.42
1:G:139:LEU:HD21	1:G:579:LEU:HD21	2.01	0.42
1:E:187:ASP:N	1:E:187:ASP:OD1	2.53	0.41
1:E:245:MET:HE2	1:E:245:MET:HA	2.01	0.41
1:G:72:ARG:HD2	1:G:146:HIS:CE1	2.54	0.41
1:G:549:TRP:CD1	1:G:564:PRO:HA	2.54	0.41
1:I:45:LYS:HA	1:I:45:LYS:HD2	1.94	0.41
1:I:182:ARG:HE	1:I:182:ARG:HA	1.84	0.41
1:J:53:TRP:HE1	1:J:649:ASN:HB2	1.84	0.41
1:K:182:ARG:NH2	1:K:563:GLN:O	2.53	0.41
1:A:297:GLY:HA2	1:A:443:VAL:O	2.20	0.41
1:C:400:VAL:HA	1:C:404:PHE:CD1	2.55	0.41
1:C:504:GLY:HA2	1:C:505:PRO:HA	1.85	0.41
1:D:372:TYR:CZ	1:D:376:ILE:HG13	2.55	0.41
1:D:428:GLY:O	1:D:432:THR:HG23	2.20	0.41
1:H:372:TYR:CZ	1:H:376:ILE:HG13	2.55	0.41
1:I:145:ARG:NH1	1:I:574:GLU:OE1	2.53	0.41
1:J:231:PRO:HG2	1:J:234:PHE:HB3	2.03	0.41
1:B:463:TRP:HB2	1:B:614:PHE:CG	2.54	0.41
1:D:471:TYR:HE2	1:D:606:ILE:HD11	1.85	0.41
1:E:378:HIS:CE1	1:E:520:ILE:HG23	2.55	0.41
1:E:605:LYS:O	1:E:609:GLU:HB3	2.20	0.41
1:F:359:MET:O	1:F:363:ARG:HG3	2.20	0.41
1:H:109:LEU:C	1:H:111:ASN:H	2.24	0.41
1:H:464:VAL:HG12	1:H:513:ILE:HG23	2.02	0.41
1:I:376:ILE:HD13	1:I:376:ILE:HA	1.95	0.41
1:J:35:PRO:CB	1:J:36:PRO:HD2	2.51	0.41
1:J:47:ASP:OD2	1:J:383:LEU:HD12	2.20	0.41
1:A:77:ARG:HE	1:A:77:ARG:HB3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:TYR:CE2	1:A:646:MET:HE1	2.54	0.41
1:D:622:GLU:HB2	1:D:641:PRO:HD2	2.01	0.41
1:F:182:ARG:HH21	1:F:561:ASP:HA	1.85	0.41
1:F:486:ALA:O	1:F:490:VAL:HG12	2.20	0.41
1:G:385:ILE:HD12	1:G:385:ILE:HA	1.92	0.41
1:I:605:LYS:O	1:I:609:GLU:HB3	2.21	0.41
1:J:358:VAL:HG11	1:J:383:LEU:HG	2.02	0.41
1:K:403:ILE:HD11	1:K:571:LEU:HG	2.02	0.41
1:K:553:PRO:N	1:K:554:PRO:HD2	2.35	0.41
1:L:241:TYR:CZ	1:L:245:MET:HG3	2.55	0.41
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.82	0.41
1:A:400:VAL:O	1:A:404:PHE:HB2	2.19	0.41
1:E:33:LEU:HD12	1:E:39:PHE:HD2	1.84	0.41
1:E:552:ALA:HB1	1:E:554:PRO:HD2	2.03	0.41
1:E:576:LEU:HD23	1:E:576:LEU:HA	1.93	0.41
1:F:330:LYS:O	1:F:334:GLN:HG2	2.20	0.41
1:F:378:HIS:CE1	1:F:520:ILE:HG23	2.55	0.41
1:F:567:GLU:HG3	1:F:567:GLU:H	1.57	0.41
1:K:369:HIS:HD2	1:K:483:GLU:OE1	2.03	0.41
1:C:92:THR:HG21	1:C:146:HIS:HB3	2.02	0.41
1:C:265:TRP:HB2	1:C:287:PRO:HD2	2.03	0.41
1:D:193:PHE:HB3	1:D:196:ILE:O	2.20	0.41
1:E:640:ILE:O	1:E:644:ILE:HG13	2.21	0.41
1:G:110:GLU:HB3	1:G:595:PHE:CE1	2.55	0.41
1:I:25:ARG:NH1	1:I:363:ARG:O	2.54	0.41
1:I:307:PRO:HB3	1:I:553:PRO:HG2	2.02	0.41
1:J:20:GLN:NE2	1:J:367:GLN:HG3	2.36	0.41
1:A:110:GLU:HB3	1:A:595:PHE:CD1	2.55	0.41
1:D:233:ASN:OD1	1:D:233:ASN:N	2.46	0.41
1:E:77:ARG:H	1:E:77:ARG:HG3	1.35	0.41
1:I:148:PRO:CB	1:I:149:PRO:HD2	2.51	0.41
1:I:602:LYS:HD3	1:I:602:LYS:HA	1.79	0.41
1:K:192:LEU:HD22	1:K:570:GLU:HB2	2.02	0.41
1:A:57:VAL:O	1:A:60:VAL:N	2.53	0.41
1:A:252:ASP:HA	1:A:255:LYS:HE3	2.03	0.41
1:A:378:HIS:CE1	1:A:520:ILE:HG23	2.56	0.41
1:A:533:PRO:HG3	1:A:638:TYR:CE2	2.55	0.41
1:D:34:LEU:HD21	1:D:412:HIS:HE1	1.86	0.41
1:E:145:ARG:H	1:E:145:ARG:HG3	1.57	0.41
1:G:486:ALA:O	1:G:490:VAL:HG12	2.20	0.41
1:H:145:ARG:NH1	1:H:574:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:PRO:HB2	1:A:126:SER:H	1.72	0.41
1:A:359:MET:O	1:A:363:ARG:HG3	2.21	0.41
1:A:372:TYR:CZ	1:A:376:ILE:HG13	2.55	0.41
1:B:316:LYS:HD2	1:B:316:LYS:HA	1.83	0.41
1:C:91:GLY:O	1:C:95:GLU:HG3	2.21	0.41
1:D:180:ASN:HA	1:D:567:GLU:HG3	2.02	0.41
1:D:408:ILE:O	1:D:412:HIS:HD2	2.04	0.41
1:H:53:TRP:CZ2	1:H:57:VAL:HG21	2.55	0.41
1:H:234:PHE:HB2	1:H:288:LEU:HD22	2.03	0.41
1:H:376:ILE:HD13	1:H:376:ILE:HA	1.90	0.41
1:I:199:PRO:HA	1:I:200:PRO:HD3	1.97	0.41
1:I:376:ILE:N	1:I:377:PRO:HD2	2.36	0.41
1:I:451:ASP:O	1:I:455:LYS:HG3	2.21	0.41
1:J:542:PRO:HA	1:J:563:GLN:OE1	2.21	0.41
1:J:579:LEU:HA	1:J:650:ILE:HG21	2.03	0.41
1:K:350:THR:OG1	1:K:351:HIS:N	2.54	0.41
1:K:585:THR:CG2	1:K:646:MET:H	2.26	0.41
1:L:21:LEU:HD23	1:L:21:LEU:HA	1.84	0.41
1:L:567:GLU:HG3	1:L:567:GLU:H	1.55	0.41
1:A:65:ALA:O	1:A:69:VAL:HG23	2.21	0.41
1:D:598:ARG:HG3	1:D:599:ALA:H	1.86	0.41
1:G:350:THR:OG1	1:G:351:HIS:N	2.54	0.41
1:H:173:ASN:N	3:H:806:HOH:O	2.53	0.41
1:I:189:TYR:CZ	1:I:563:GLN:HB2	2.56	0.41
1:B:139:LEU:HD22	1:B:393:LEU:HD13	2.03	0.40
1:F:429:LEU:O	1:F:433:ILE:HG12	2.20	0.40
1:H:403:ILE:HD11	1:H:571:LEU:HG	2.02	0.40
1:H:429:LEU:O	1:H:433:ILE:HG12	2.21	0.40
1:J:40:CYS:HB2	1:J:383:LEU:HD22	2.01	0.40
1:J:396:PRO:HG3	1:J:408:ILE:HG21	2.03	0.40
1:J:585:THR:CG2	1:J:646:MET:H	2.33	0.40
1:K:45:LYS:HD2	1:K:45:LYS:HA	1.85	0.40
1:L:273:VAL:O	1:L:407:THR:HG23	2.21	0.40
1:B:21:LEU:HD23	1:B:21:LEU:HA	1.96	0.40
1:E:10:ASN:HB3	1:J:203:SER:O	2.20	0.40
1:F:287:PRO:HG2	1:F:333:VAL:HA	2.03	0.40
1:H:640:ILE:O	1:H:644:ILE:HG13	2.22	0.40
1:J:383:LEU:HD23	1:J:383:LEU:HA	1.95	0.40
1:J:576:LEU:HD23	1:J:576:LEU:HA	1.92	0.40
1:L:335:VAL:HA	1:L:545:THR:O	2.21	0.40
1:L:622:GLU:HB2	1:L:641:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:TYR:HB3	1:A:215:ARG:NH1	2.36	0.40
1:A:244:ALA:HB2	1:A:320:THR:OG1	2.21	0.40
1:C:4:ILE:HA	1:C:5:PRO:HD3	1.98	0.40
1:I:35:PRO:CB	1:I:36:PRO:HD2	2.51	0.40
1:K:624:LEU:HD12	1:K:624:LEU:HA	1.93	0.40
1:A:249:ASP:OD1	1:A:250:SER:N	2.50	0.40
1:B:144:ASN:O	1:B:144:ASN:ND2	2.53	0.40
1:D:277:TYR:OH	1:D:567:GLU:OE1	2.25	0.40
1:E:277:TYR:HB2	1:E:282:LYS:HD2	2.03	0.40
1:I:21:LEU:HB3	1:I:25:ARG:NH2	2.37	0.40
1:K:239:ALA:O	1:K:243:GLN:HG3	2.22	0.40
1:K:376:ILE:HD13	1:K:376:ILE:HA	1.92	0.40
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.89	0.40
1:C:605:LYS:O	1:C:609:GLU:HB3	2.21	0.40
1:I:318:TYR:CE1	1:I:325:ASP:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/650 (92%)	558 (93%)	33 (6%)	8 (1%)	10	32
1	B	592/650 (91%)	558 (94%)	29 (5%)	5 (1%)	16	44
1	C	594/650 (91%)	559 (94%)	33 (6%)	2 (0%)	37	67
1	D	599/650 (92%)	569 (95%)	23 (4%)	7 (1%)	11	34
1	E	596/650 (92%)	562 (94%)	27 (4%)	7 (1%)	11	34
1	F	597/650 (92%)	559 (94%)	32 (5%)	6 (1%)	13	39
1	G	595/650 (92%)	564 (95%)	25 (4%)	6 (1%)	13	39
1	H	596/650 (92%)	555 (93%)	37 (6%)	4 (1%)	19	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	595/650 (92%)	568 (96%)	23 (4%)	4 (1%)	19	48
1	J	596/650 (92%)	562 (94%)	30 (5%)	4 (1%)	19	48
1	K	592/650 (91%)	559 (94%)	30 (5%)	3 (0%)	25	56
1	L	592/650 (91%)	565 (95%)	24 (4%)	3 (0%)	25	56
All	All	7143/7800 (92%)	6738 (94%)	346 (5%)	59 (1%)	16	44

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	PRO
1	A	149	PRO
1	A	585	THR
1	B	36	PRO
1	B	585	THR
1	C	36	PRO
1	C	149	PRO
1	D	36	PRO
1	D	125	PRO
1	D	149	PRO
1	E	36	PRO
1	E	149	PRO
1	F	36	PRO
1	F	125	PRO
1	F	149	PRO
1	G	36	PRO
1	G	149	PRO
1	H	36	PRO
1	H	149	PRO
1	I	36	PRO
1	I	149	PRO
1	J	36	PRO
1	J	149	PRO
1	K	36	PRO
1	K	149	PRO
1	L	36	PRO
1	L	149	PRO
1	D	112	PHE
1	H	175	SER
1	I	585	THR
1	G	585	THR
1	J	585	THR

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Mol	Chain	Res	Type
1	A	106	LEU
1	A	143	PRO
1	D	554	PRO
1	E	554	PRO
1	E	585	THR
1	G	550	THR
1	H	585	THR
1	I	554	PRO
1	L	585	THR
1	E	609	GLU
1	F	148	PRO
1	F	585	THR
1	G	148	PRO
1	A	110	GLU
1	A	128	LEU
1	A	219	PRO
1	D	150	ALA
1	E	344	VAL
1	B	554	PRO
1	B	307	PRO
1	G	554	PRO
1	J	554	PRO
1	E	505	PRO
1	B	505	PRO
1	K	505	PRO
1	D	505	PRO
1	F	505	PRO

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	484/518 (93%)	443 (92%)	41 (8%)	8 27
1	B	480/518 (93%)	448 (93%)	32 (7%)	13 38
1	C	481/518 (93%)	447 (93%)	34 (7%)	12 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	486/518 (94%)	452 (93%)	34 (7%)	12 36
1	E	483/518 (93%)	445 (92%)	38 (8%)	10 30
1	F	484/518 (93%)	457 (94%)	27 (6%)	17 47
1	G	482/518 (93%)	445 (92%)	37 (8%)	10 31
1	H	483/518 (93%)	456 (94%)	27 (6%)	17 47
1	I	482/518 (93%)	451 (94%)	31 (6%)	14 41
1	J	483/518 (93%)	450 (93%)	33 (7%)	13 38
1	K	479/518 (92%)	451 (94%)	28 (6%)	17 45
1	L	478/518 (92%)	452 (95%)	26 (5%)	18 48
All	All	5785/6216 (93%)	5397 (93%)	388 (7%)	13 38

All (388) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	13	ARG
1	A	15	GLU
1	A	22	ASP
1	A	39	PHE
1	A	64	VAL
1	A	76	LYS
1	A	77	ARG
1	A	87	PHE
1	A	88	ASP
1	A	89	VAL
1	A	94	GLU
1	A	105	PHE
1	A	109	LEU
1	A	127	VAL
1	A	215	ARG
1	A	222	SER
1	A	252	ASP
1	A	272	LEU
1	A	283	THR
1	A	299	SER
1	A	314	THR
1	A	320	THR
1	A	337	GLU
1	A	409	GLU

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Mol	Chain	Res	Type
1	A	419	LEU
1	A	421	ARG
1	A	425	MET
1	A	447	TYR
1	A	454	LEU
1	A	473	ILE
1	A	479	THR
1	A	501	SER
1	A	567	GLU
1	A	593	ASN
1	A	595	PHE
1	A	607	THR
1	A	617	ASP
1	A	626	VAL
1	A	643	THR
1	A	650	ILE
1	B	27	THR
1	B	34	LEU
1	B	39	PHE
1	B	47	ASP
1	B	76	LYS
1	B	87	PHE
1	B	105	PHE
1	B	109	LEU
1	B	127	VAL
1	B	146	HIS
1	B	209	SER
1	B	215	ARG
1	B	223	MET
1	B	229	GLU
1	B	262	LEU
1	B	272	LEU
1	B	310	THR
1	B	314	THR
1	B	320	THR
1	B	407	THR
1	B	409	GLU
1	B	425	MET
1	B	447	TYR
1	B	490	VAL
1	B	522	THR
1	B	567	GLU

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Mol	Chain	Res	Type
1	B	607	THR
1	B	610	LEU
1	B	633	THR
1	B	646	MET
1	B	649	ASN
1	B	650	ILE
1	C	6	THR
1	C	13	ARG
1	C	15	GLU
1	C	34	LEU
1	C	41	GLU
1	C	48	THR
1	C	87	PHE
1	C	88	ASP
1	C	89	VAL
1	C	94	GLU
1	C	98	ASN
1	C	127	VAL
1	C	147	VAL
1	C	184	GLN
1	C	187	ASP
1	C	209	SER
1	C	215	ARG
1	C	225	GLN
1	C	229	GLU
1	C	252	ASP
1	C	299	SER
1	C	320	THR
1	C	425	MET
1	C	444	LEU
1	C	447	TYR
1	C	556	GLN
1	C	567	GLU
1	C	575	PHE
1	C	585	THR
1	C	593	ASN
1	C	600	TRP
1	C	610	LEU
1	C	617	ASP
1	C	650	ILE
1	D	33	LEU
1	D	34	LEU

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Mol	Chain	Res	Type
1	D	39	PHE
1	D	41	GLU
1	D	47	ASP
1	D	48	THR
1	D	77	ARG
1	D	105	PHE
1	D	127	VAL
1	D	145	ARG
1	D	147	VAL
1	D	187	ASP
1	D	215	ARG
1	D	219	PRO
1	D	228	THR
1	D	236	VAL
1	D	272	LEU
1	D	274	ASN
1	D	316	LYS
1	D	320	THR
1	D	343	LEU
1	D	409	GLU
1	D	425	MET
1	D	441	THR
1	D	447	TYR
1	D	473	ILE
1	D	507	ASP
1	D	522	THR
1	D	545	THR
1	D	567	GLU
1	D	575	PHE
1	D	585	THR
1	D	622	GLU
1	D	631	THR
1	E	22	ASP
1	E	27	THR
1	E	39	PHE
1	E	47	ASP
1	E	48	THR
1	E	75	TRP
1	E	77	ARG
1	E	87	PHE
1	E	89	VAL
1	E	94	GLU

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Mol	Chain	Res	Type
1	E	99	GLU
1	E	102	HIS
1	E	105	PHE
1	E	127	VAL
1	E	145	ARG
1	E	176	LYS
1	E	187	ASP
1	E	204	THR
1	E	215	ARG
1	E	222	SER
1	E	228	THR
1	E	247	GLU
1	E	314	THR
1	E	316	LYS
1	E	331	SER
1	E	343	LEU
1	E	409	GLU
1	E	425	MET
1	E	441	THR
1	E	447	TYR
1	E	567	GLU
1	E	575	PHE
1	E	585	THR
1	E	595	PHE
1	E	600	TRP
1	E	624	LEU
1	E	637	THR
1	E	650	ILE
1	F	32	ASP
1	F	87	PHE
1	F	89	VAL
1	F	94	GLU
1	F	106	LEU
1	F	144	ASN
1	F	145	ARG
1	F	187	ASP
1	F	204	THR
1	F	215	ARG
1	F	223	MET
1	F	233	ASN
1	F	249	ASP
1	F	276	THR

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Mol	Chain	Res	Type
1	F	320	THR
1	F	409	GLU
1	F	425	MET
1	F	447	TYR
1	F	461	GLU
1	F	490	VAL
1	F	522	THR
1	F	567	GLU
1	F	575	PHE
1	F	585	THR
1	F	600	TRP
1	F	642	SER
1	F	650	ILE
1	G	39	PHE
1	G	47	ASP
1	G	77	ARG
1	G	89	VAL
1	G	103	ASN
1	G	105	PHE
1	G	127	VAL
1	G	144	ASN
1	G	147	VAL
1	G	180	ASN
1	G	184	GLN
1	G	204	THR
1	G	215	ARG
1	G	222	SER
1	G	228	THR
1	G	233	ASN
1	G	236	VAL
1	G	238	ASP
1	G	245	MET
1	G	283	THR
1	G	288	LEU
1	G	310	THR
1	G	316	LYS
1	G	409	GLU
1	G	425	MET
1	G	447	TYR
1	G	463	TRP
1	G	473	ILE
1	G	522	THR

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Mol	Chain	Res	Type
1	G	535	LYS
1	G	560	LYS
1	G	567	GLU
1	G	585	THR
1	G	593	ASN
1	G	600	TRP
1	G	637	THR
1	G	643	THR
1	H	3	ASN
1	H	6	THR
1	H	76	LYS
1	H	127	VAL
1	H	187	ASP
1	H	215	ARG
1	H	234	PHE
1	H	247	GLU
1	H	299	SER
1	H	310	THR
1	H	314	THR
1	H	331	SER
1	H	407	THR
1	H	425	MET
1	H	442	SER
1	H	447	TYR
1	H	535	LYS
1	H	556	GLN
1	H	567	GLU
1	H	575	PHE
1	H	585	THR
1	H	598	ARG
1	H	600	TRP
1	H	610	LEU
1	H	617	ASP
1	H	629	ASN
1	H	650	ILE
1	I	6	THR
1	I	32	ASP
1	I	39	PHE
1	I	48	THR
1	I	95	GLU
1	I	127	VAL
1	I	146	HIS

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Mol	Chain	Res	Type
1	I	147	VAL
1	I	182	ARG
1	I	204	THR
1	I	215	ARG
1	I	222	SER
1	I	234	PHE
1	I	236	VAL
1	I	310	THR
1	I	321	GLN
1	I	331	SER
1	I	421	ARG
1	I	434	GLU
1	I	447	TYR
1	I	490	VAL
1	I	539	SER
1	I	575	PHE
1	I	607	THR
1	I	610	LEU
1	I	617	ASP
1	I	633	THR
1	I	634	PHE
1	I	642	SER
1	I	649	ASN
1	I	650	ILE
1	J	34	LEU
1	J	39	PHE
1	J	87	PHE
1	J	89	VAL
1	J	94	GLU
1	J	98	ASN
1	J	102	HIS
1	J	112	PHE
1	J	128	LEU
1	J	176	LYS
1	J	187	ASP
1	J	215	ARG
1	J	228	THR
1	J	236	VAL
1	J	249	ASP
1	J	268	ILE
1	J	314	THR
1	J	316	LYS

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Mol	Chain	Res	Type
1	J	409	GLU
1	J	447	TYR
1	J	490	VAL
1	J	539	SER
1	J	556	GLN
1	J	567	GLU
1	J	575	PHE
1	J	585	THR
1	J	598	ARG
1	J	600	TRP
1	J	610	LEU
1	J	617	ASP
1	J	635	LYS
1	J	649	ASN
1	J	650	ILE
1	K	6	THR
1	K	22	ASP
1	K	32	ASP
1	K	48	THR
1	K	50	SER
1	K	94	GLU
1	K	106	LEU
1	K	127	VAL
1	K	184	GLN
1	K	187	ASP
1	K	204	THR
1	K	215	ARG
1	K	234	PHE
1	K	247	GLU
1	K	310	THR
1	K	320	THR
1	K	343	LEU
1	K	425	MET
1	K	447	TYR
1	K	535	LYS
1	K	567	GLU
1	K	575	PHE
1	K	585	THR
1	K	600	TRP
1	K	607	THR
1	K	617	ASP
1	K	622	GLU

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Mol	Chain	Res	Type
1	K	643	THR
1	L	6	THR
1	L	22	ASP
1	L	33	LEU
1	L	47	ASP
1	L	88	ASP
1	L	89	VAL
1	L	94	GLU
1	L	176	LYS
1	L	187	ASP
1	L	203	SER
1	L	215	ARG
1	L	222	SER
1	L	225	GLN
1	L	229	GLU
1	L	247	GLU
1	L	314	THR
1	L	316	LYS
1	L	320	THR
1	L	425	MET
1	L	438	VAL
1	L	447	TYR
1	L	567	GLU
1	L	585	THR
1	L	600	TRP
1	L	610	LEU
1	L	624	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	220	ASN
1	C	477	ASN
1	C	531	ASN
1	C	534	GLN
1	D	459	ASN
1	D	531	ASN
1	E	459	ASN
1	G	173	ASN
1	G	477	ASN
1	K	531	ASN
1	L	346	HIS

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Mol	Chain	Res	Type
1	L	534	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

Of 48 ligands modelled in this entry, 48 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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.