



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:53 AM EDT

PDB ID : 9LU2 / pdb_00009lu2
Title : Crystal structure of Pseudoalteromonas sp. L11-2 tryptophan halogenase putative
Authors : Arold, S.T.; Hameed, U.F.S.
Deposited on : 2025-02-07
Resolution : 2.98 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

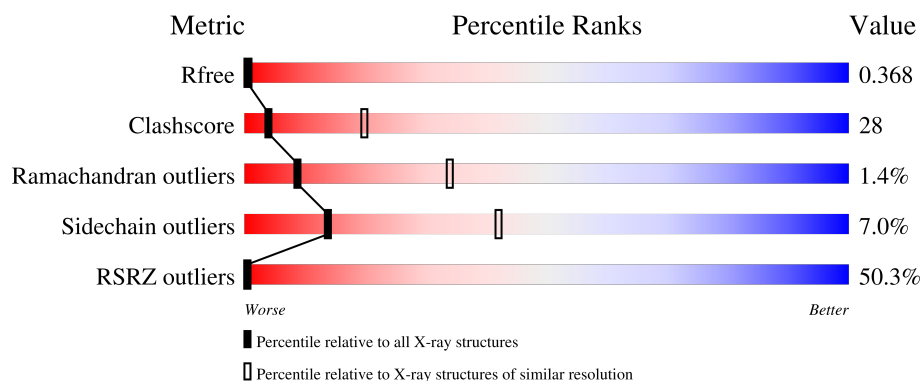
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	514	46% 53% 34% 5% 6%
1	B	514	49% 49% 40% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7679 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.

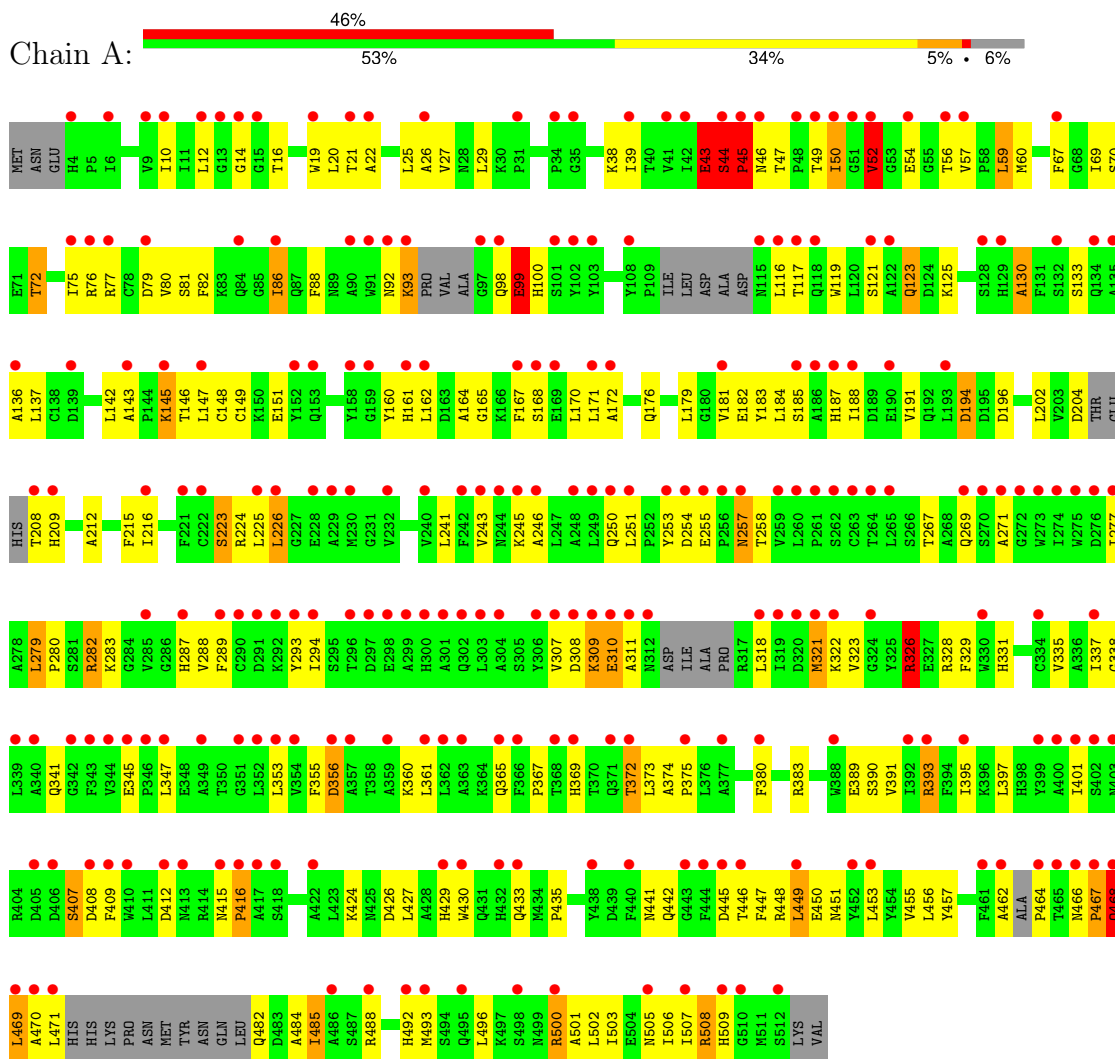
- Molecule 1 is a protein called L11-2 tryptophan halogenase putative.

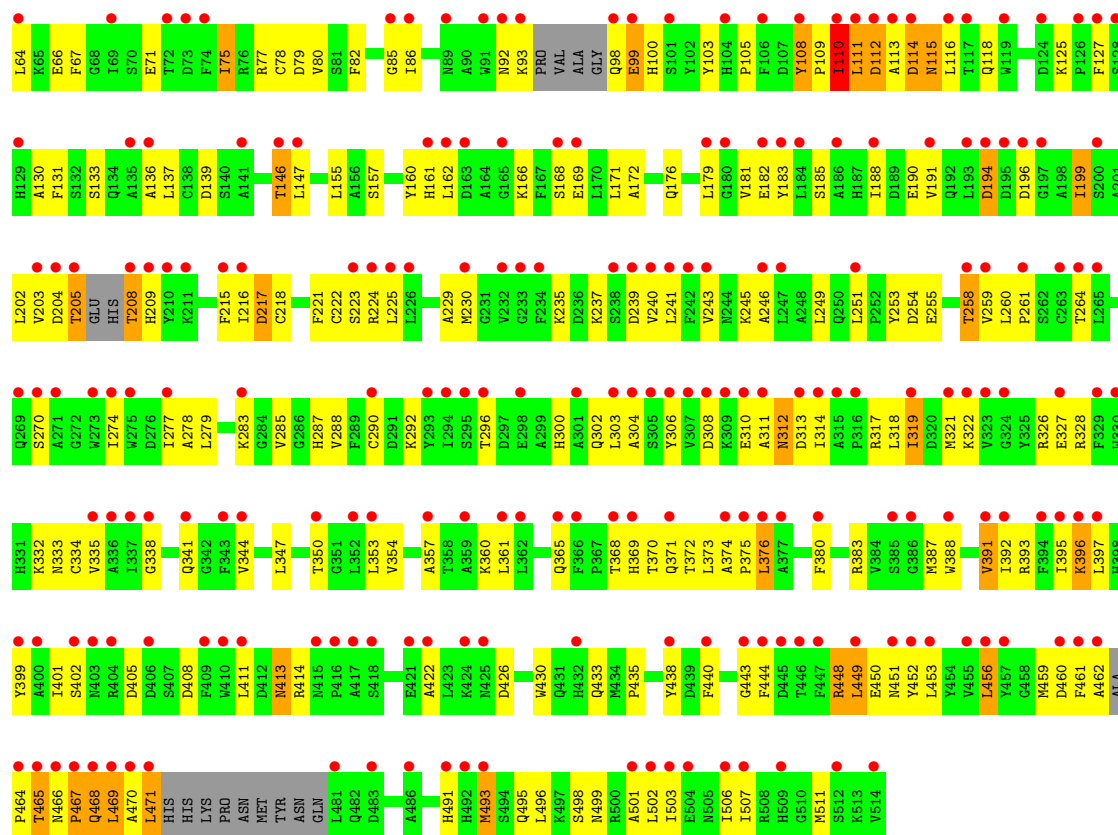
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3801	2424	653	707	17			
1	B	493	Total	C	N	O	S	0	0	0
			3878	2473	663	725	17			

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 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: L11-2 tryptophan halogenase putative





4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.90Å 63.16Å 214.08Å 90.00° 99.81° 90.00°	Depositor
Resolution (Å)	47.91 – 2.98 47.91 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.91-2.98) 98.0 (47.91-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.01Å)	Xtriage
Refinement program	REFMAC refmac5	Depositor
R, R_{free}	0.322 , 0.365 0.335 , 0.368	Depositor DCC
R_{free} test set	1158 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	7679	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.66	3/3898 (0.1%)	1.32	41/5288 (0.8%)
1	B	0.66	3/3976 (0.1%)	1.27	30/5397 (0.6%)
All	All	0.66	6/7874 (0.1%)	1.29	71/10685 (0.7%)

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	5
1	B	0	5
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	PRO	N-CD	9.89	1.61	1.47
1	A	321	MET	SD-CE	-6.32	1.63	1.79
1	A	407	SER	C-N	-6.25	1.24	1.33
1	B	199	ILE	CG1-CD1	-6.18	1.27	1.51
1	B	75	ILE	CG1-CD1	-5.65	1.29	1.51
1	B	493	MET	SD-CE	-5.51	1.65	1.79

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	GLN	N-CA-C	24.32	137.79	111.28
1	B	46	ASN	N-CA-C	-21.75	74.92	109.72
1	B	34	PRO	CB-CA-C	-21.52	76.06	111.56
1	A	321	MET	CB-CA-C	-18.17	74.27	110.42
1	B	469	LEU	N-CA-C	16.99	135.30	111.52
1	A	408	ASP	N-CA-C	-16.64	93.03	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	PRO	N-CA-C	14.26	141.85	112.47
1	A	310	GLU	N-CA-C	13.98	140.59	110.80
1	B	470	ALA	N-CA-C	13.82	132.70	111.56
1	A	100	HIS	N-CA-CB	13.67	130.33	110.37
1	A	322	LYS	N-CA-CB	-13.47	88.44	109.19
1	A	310	GLU	CB-CA-C	-12.78	84.98	110.42
1	A	416	PRO	CB-CA-C	11.72	130.90	111.56
1	B	46	ASN	CB-CA-C	10.79	130.58	109.33
1	A	467	PRO	CB-CA-C	-10.58	97.85	111.39
1	B	35	GLY	N-CA-C	-10.16	89.11	113.18
1	A	99	GLU	N-CA-C	-9.83	93.62	108.46
1	A	309	LYS	N-CA-C	-9.28	91.78	108.02
1	A	470	ALA	N-CA-C	-8.22	96.04	108.46
1	A	223	SER	N-CA-C	8.21	121.28	111.02
1	A	467	PRO	N-CA-C	7.86	123.61	111.11
1	B	99	GLU	N-CA-CB	-7.80	98.83	111.24
1	B	449	LEU	N-CA-C	7.75	119.37	111.07
1	A	470	ALA	CB-CA-C	7.65	122.03	109.72
1	A	308	ASP	CB-CA-C	-7.24	99.56	111.36
1	A	321	MET	N-CA-C	7.17	126.07	110.80
1	B	47	THR	N-CA-CB	-7.09	101.17	110.17
1	B	28	ASN	N-CA-C	7.07	121.14	112.23
1	B	7	GLN	N-CA-C	6.89	121.35	113.15
1	B	310	GLU	N-CA-C	6.83	121.33	111.56
1	A	468	GLN	CB-CA-C	-6.79	99.52	110.79
1	A	469	LEU	N-CA-CB	6.74	122.12	111.20
1	A	148	CYS	N-CA-C	-6.63	105.22	113.38
1	A	148	CYS	CB-CA-C	6.43	120.84	109.65
1	B	112	ASP	CB-CA-C	-6.43	109.15	116.54
1	B	449	LEU	CB-CA-C	-6.42	100.79	110.88
1	A	449	LEU	N-CA-C	6.39	124.41	110.80
1	B	470	ALA	CB-CA-C	-6.37	99.13	111.03
1	A	322	LYS	N-CA-C	6.27	119.92	110.64
1	B	100	HIS	N-CA-CB	6.24	120.61	110.32
1	B	194	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	471	LEU	N-CA-CB	-6.12	100.10	110.50
1	A	468	GLN	N-CA-CB	-6.09	101.17	110.12
1	A	469	LEU	N-CA-C	-6.07	100.27	109.85
1	A	43	GLU	CA-C-O	-6.06	114.93	121.36
1	A	407	SER	O-C-N	-6.06	114.53	122.59
1	B	467	PRO	CB-CA-C	5.92	121.33	111.56
1	A	254	ASP	CA-CB-CG	5.83	118.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	MET	N-CA-C	-5.79	106.45	112.93
1	A	194	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	507	ILE	N-CA-C	-5.74	97.39	109.34
1	A	99	GLU	CB-CA-C	5.71	118.92	109.72
1	A	311	ALA	N-CA-C	5.45	122.41	110.80
1	A	44	SER	C-N-CD	-5.45	102.67	125.00
1	B	108	TYR	N-CA-CB	-5.41	101.87	110.03
1	B	461	PHE	CA-CB-CG	5.35	119.15	113.80
1	B	110	ILE	N-CA-C	5.34	120.45	109.34
1	B	108	TYR	CB-CA-C	5.33	118.20	109.46
1	A	204	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	424	LYS	CB-CA-C	-5.28	101.97	110.74
1	A	356	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	26	ALA	N-CA-C	-5.23	103.13	110.35
1	A	309	LYS	N-CA-CB	5.23	118.91	110.65
1	B	413	ASN	N-CA-C	-5.22	106.87	113.18
1	A	507	ILE	CB-CA-C	5.16	119.75	111.29
1	A	130	ALA	N-CA-C	-5.13	104.10	110.41
1	A	372	THR	CA-CB-OG1	-5.13	101.91	109.60
1	B	45	PRO	N-CA-C	-5.12	98.94	112.92
1	B	218	CYS	CB-CA-C	5.08	117.53	111.22
1	B	217	ASP	N-CA-C	5.06	118.37	111.39
1	B	300	HIS	CA-CB-CG	5.02	118.82	113.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	407	SER	Mainchain
1	A	500	ARG	Sidechain
1	B	224	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	328	ARG	Sidechain
1	B	414	ARG	Sidechain
1	B	448	ARG	Sidechain

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	3801	0	3668	207	2
1	B	3878	0	3748	223	3
All	All	7679	0	7416	424	3

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 28.

All (424) 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:B:108:TYR:HE1	1:B:448:ARG:NH2	1.27	1.32
1:B:108:TYR:CE1	1:B:448:ARG:NH2	2.15	1.14
1:B:369:HIS:CE1	1:B:371:GLN:HB3	1.90	1.07
1:A:449:LEU:O	1:A:453:LEU:HB2	1.53	1.07
1:B:217:ASP:OD2	1:B:223:SER:OG	1.72	1.06
1:B:240:VAL:HG12	1:B:241:LEU:HD22	1.39	1.01
1:B:127:PHE:CZ	1:B:453:LEU:CD2	2.46	0.99
1:B:208:THR:HG22	1:B:209:HIS:H	1.29	0.96
1:A:390:SER:OG	1:A:446:THR:OG1	1.82	0.94
1:B:108:TYR:HE1	1:B:448:ARG:HH21	1.15	0.93
1:A:243:VAL:HG11	1:A:288:VAL:HG12	1.46	0.93
1:B:449:LEU:O	1:B:453:LEU:HB2	1.67	0.93
1:A:39:ILE:HG22	1:A:181:VAL:HG13	1.48	0.93
1:A:243:VAL:HG11	1:A:288:VAL:CG1	1.99	0.92
1:A:188:ILE:HD11	1:A:224:ARG:HG2	1.46	0.92
1:B:127:PHE:CZ	1:B:453:LEU:HD21	2.06	0.91
1:A:12:LEU:HD11	1:A:188:ILE:HD13	1.51	0.91
1:A:168:SER:HA	1:A:171:LEU:HD12	1.54	0.90
1:A:75:ILE:HG21	1:A:506:ILE:CG2	2.02	0.89
1:A:75:ILE:HG21	1:A:506:ILE:HG22	1.55	0.89
1:A:72:THR:O	1:A:75:ILE:HG22	1.73	0.88
1:B:237:LYS:HZ2	1:B:392:ILE:HD13	1.40	0.85
1:B:57:VAL:HG21	1:B:353:LEU:HD13	1.58	0.84
1:A:16:THR:O	1:A:20:LEU:HG	1.77	0.84
1:B:26:ALA:O	1:B:27:VAL:HG22	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:TYR:HE1	1:B:448:ARG:HH22	1.22	0.84
1:B:75:ILE:HD12	1:B:506:ILE:HG21	1.62	0.82
1:A:12:LEU:HD22	1:A:225:LEU:HD11	1.61	0.81
1:B:288:VAL:HG13	1:B:321:MET:HE1	1.64	0.80
1:B:208:THR:HG22	1:B:209:HIS:N	1.97	0.80
1:A:255:GLU:HG2	1:A:258:THR:CG2	2.12	0.79
1:A:255:GLU:HG2	1:A:258:THR:HG22	1.63	0.79
1:A:143:ALA:O	1:A:496:LEU:HD13	1.83	0.78
1:A:25:LEU:HD12	1:A:29:LEU:CD1	2.14	0.78
1:A:133:SER:O	1:A:137:LEU:HD13	1.83	0.77
1:A:329:PHE:CD1	1:A:341:GLN:HG3	2.20	0.75
1:A:466:ASN:HD22	1:B:368:THR:HG22	1.50	0.75
1:A:44:SER:N	1:A:45:PRO:HD2	2.02	0.75
1:A:462:ALA:C	1:A:464:PRO:N	2.45	0.75
1:A:136:ALA:HB1	1:A:493:MET:HE1	1.69	0.75
1:B:93:LYS:HE2	1:B:99:GLU:H	1.52	0.75
1:A:241:LEU:CD1	1:A:323:VAL:HG11	2.17	0.74
1:B:237:LYS:NZ	1:B:392:ILE:HD13	2.02	0.74
1:B:350:THR:HG21	1:B:391:VAL:CG1	2.17	0.74
1:A:39:ILE:CG2	1:A:181:VAL:HG13	2.18	0.73
1:B:498:SER:OG	1:B:501:ALA:CB	2.36	0.73
1:B:217:ASP:CG	1:B:223:SER:OG	2.29	0.73
1:B:176:GLN:HE21	1:B:183:TYR:HB2	1.54	0.73
1:B:215:PHE:HE1	1:B:333:ASN:ND2	1.87	0.73
1:B:246:ALA:HB3	1:B:319:ILE:HG23	1.70	0.72
1:A:367:PRO:CG	1:A:373:LEU:CD2	2.68	0.72
1:A:433:GLN:HE22	1:B:365:GLN:HA	1.53	0.71
1:A:255:GLU:O	1:A:258:THR:HG23	1.91	0.71
1:B:240:VAL:HG12	1:B:241:LEU:CD2	2.17	0.71
1:B:369:HIS:CE1	1:B:371:GLN:CB	2.72	0.71
1:B:6:ILE:O	1:B:6:ILE:HG22	1.90	0.71
1:B:304:ALA:HB1	1:B:311:ALA:H	1.56	0.70
1:B:208:THR:CG2	1:B:209:HIS:N	2.54	0.70
1:A:288:VAL:HG13	1:A:321:MET:HE1	1.73	0.70
1:B:127:PHE:CZ	1:B:453:LEU:HD22	2.26	0.70
1:B:59:LEU:HD12	1:B:62:HIS:HB3	1.71	0.70
1:A:59:LEU:HD21	1:A:356:ASP:OD2	1.90	0.70
1:A:12:LEU:HD22	1:A:225:LEU:HD21	1.73	0.70
1:A:25:LEU:HD12	1:A:29:LEU:HD12	1.74	0.70
1:A:288:VAL:HG22	1:A:321:MET:HE1	1.74	0.69
1:B:199:ILE:HG22	1:B:215:PHE:CZ	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:CB	1:A:373:LEU:HD21	2.23	0.68
1:A:12:LEU:HD22	1:A:225:LEU:CG	2.23	0.68
1:A:12:LEU:HD22	1:A:225:LEU:CD1	2.23	0.68
1:B:39:ILE:HG22	1:B:181:VAL:HG13	1.76	0.68
1:A:161:HIS:CD2	1:A:277:ILE:HG23	2.28	0.68
1:A:241:LEU:HD13	1:A:323:VAL:HG11	1.76	0.68
1:A:70:SER:OG	1:A:151:GLU:OE2	2.12	0.67
1:B:16:THR:HG22	1:B:168:SER:OG	1.94	0.67
1:B:191:VAL:HG22	1:B:202:LEU:HD22	1.77	0.67
1:A:75:ILE:HG21	1:A:506:ILE:HG21	1.77	0.67
1:A:367:PRO:CG	1:A:373:LEU:HD21	2.25	0.67
1:A:52:VAL:HG11	1:A:250:GLN:HG2	1.77	0.66
1:B:237:LYS:NZ	1:B:392:ILE:CD1	2.58	0.66
1:A:367:PRO:HB3	1:A:373:LEU:HD23	1.76	0.66
1:B:239:ASP:OD1	1:B:240:VAL:HG23	1.95	0.66
1:B:60:MET:O	1:B:64:LEU:HD12	1.96	0.66
1:A:45:PRO:HB3	1:A:187:HIS:CD2	2.30	0.66
1:A:442:GLN:OE1	1:A:445:ASP:OD1	2.12	0.66
1:A:367:PRO:CB	1:A:373:LEU:CD2	2.74	0.66
1:B:161:HIS:CD2	1:B:277:ILE:HG23	2.31	0.66
1:B:199:ILE:HB	1:B:215:PHE:CE1	2.32	0.65
1:B:208:THR:CG2	1:B:209:HIS:H	2.07	0.65
1:A:367:PRO:HG2	1:A:373:LEU:HD21	1.79	0.64
1:B:127:PHE:HZ	1:B:453:LEU:HD21	1.58	0.64
1:A:361:LEU:HD23	1:A:380:PHE:CE1	2.32	0.64
1:B:136:ALA:HB1	1:B:493:MET:CE	2.27	0.64
1:B:215:PHE:HE1	1:B:333:ASN:HD21	1.42	0.64
1:B:7:GLN:HG3	1:B:36:GLY:O	1.98	0.64
1:A:338:GLY:HA2	1:A:355:PHE:CE1	2.32	0.64
1:A:56:THR:OG1	1:A:160:TYR:N	2.28	0.64
1:A:82:PHE:CE2	1:A:502:LEU:HD23	2.33	0.63
1:B:387:MET:O	1:B:391:VAL:HG23	1.98	0.63
1:A:255:GLU:CG	1:A:258:THR:HG22	2.28	0.63
1:B:216:ILE:O	1:B:335:VAL:O	2.17	0.62
1:B:75:ILE:CD1	1:B:506:ILE:HG21	2.27	0.62
1:A:59:LEU:HD23	1:A:59:LEU:C	2.25	0.61
1:A:70:SER:HG	1:A:151:GLU:CD	2.08	0.61
1:B:468:GLN:HG2	1:B:469:LEU:H	1.65	0.61
1:A:59:LEU:CD2	1:A:356:ASP:OD2	2.48	0.61
1:A:72:THR:O	1:A:75:ILE:CG2	2.47	0.61
1:A:208:THR:HG22	1:A:209:HIS:ND1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PHE:CE1	1:B:453:LEU:HD22	2.35	0.61
1:A:44:SER:N	1:A:45:PRO:CD	2.63	0.61
1:A:79:ASP:O	1:A:279:LEU:CD2	2.49	0.61
1:B:56:THR:OG1	1:B:160:TYR:N	2.27	0.61
1:B:448:ARG:HG2	1:B:449:LEU:H	1.65	0.61
1:B:92:ASN:HD21	1:B:402:SER:HA	1.65	0.61
1:A:86:ILE:HG12	1:A:88:PHE:CE1	2.35	0.60
1:B:59:LEU:HD21	1:B:360:LYS:HE3	1.83	0.60
1:B:39:ILE:CG2	1:B:181:VAL:HG13	2.32	0.60
1:A:25:LEU:HD12	1:A:29:LEU:HD11	1.84	0.60
1:A:246:ALA:HB2	1:A:321:MET:CE	2.32	0.60
1:B:498:SER:OG	1:B:501:ALA:HB2	2.00	0.60
1:A:12:LEU:HD22	1:A:225:LEU:CD2	2.32	0.59
1:B:240:VAL:HG13	1:B:396:LYS:HG3	1.83	0.59
1:A:442:GLN:HB3	1:A:445:ASP:CG	2.27	0.59
1:B:204:ASP:O	1:B:205:THR:HG22	2.02	0.59
1:B:240:VAL:CG1	1:B:241:LEU:HD22	2.24	0.59
1:B:6:ILE:HG13	1:B:369:HIS:HA	1.85	0.59
1:B:60:MET:O	1:B:64:LEU:CD1	2.51	0.58
1:A:456:LEU:HD23	1:A:457:TYR:CE1	2.39	0.58
1:B:92:ASN:ND2	1:B:402:SER:HA	2.18	0.58
1:B:393:ARG:NE	1:B:422:ALA:HB3	2.18	0.58
1:A:367:PRO:HG2	1:A:373:LEU:CD2	2.34	0.58
1:A:54:GLU:HG3	1:A:164:ALA:HB2	1.86	0.58
1:A:39:ILE:HG22	1:A:181:VAL:CG1	2.28	0.58
1:B:78:CYS:HA	1:B:166:LYS:HB2	1.86	0.58
1:B:188:ILE:HD13	1:B:202:LEU:HD13	1.85	0.58
1:B:215:PHE:CE1	1:B:333:ASN:ND2	2.69	0.58
1:B:347:LEU:HB3	1:B:395:ILE:HD12	1.84	0.58
1:B:354:VAL:HG11	1:B:388:TRP:CZ2	2.39	0.57
1:B:176:GLN:HE21	1:B:183:TYR:CB	2.18	0.57
1:B:503:ILE:O	1:B:507:ILE:HG12	2.04	0.57
1:A:12:LEU:HD13	1:A:202:LEU:HD13	1.86	0.57
1:A:367:PRO:HB3	1:A:373:LEU:CD2	2.33	0.57
1:B:115:ASN:O	1:B:116:LEU:C	2.46	0.57
1:A:255:GLU:HG2	1:A:258:THR:HG23	1.87	0.57
1:B:462:ALA:C	1:B:464:PRO:N	2.63	0.57
1:B:19:TRP:HB3	1:B:171:LEU:HB3	1.86	0.57
1:A:75:ILE:HA	1:A:80:VAL:HB	1.86	0.56
1:B:237:LYS:HZ1	1:B:392:ILE:CD1	2.18	0.56
1:B:133:SER:O	1:B:137:LEU:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HD21	1:B:251:LEU:HD21	1.87	0.56
1:A:241:LEU:HD12	1:A:323:VAL:HG11	1.88	0.56
1:A:412:ASP:HA	1:A:415:ASN:HD22	1.71	0.56
1:A:433:GLN:NE2	1:B:365:GLN:HA	2.20	0.56
1:B:75:ILE:HA	1:B:80:VAL:HB	1.88	0.56
1:B:408:ASP:HA	1:B:411:LEU:HB2	1.88	0.56
1:B:304:ALA:CB	1:B:311:ALA:H	2.19	0.56
1:B:350:THR:CG2	1:B:391:VAL:CG1	2.83	0.56
1:A:59:LEU:HD21	1:A:356:ASP:CG	2.31	0.55
1:B:361:LEU:HD23	1:B:380:PHE:CE1	2.40	0.55
1:A:45:PRO:HG2	1:A:46:ASN:H	1.71	0.55
1:A:243:VAL:HG11	1:A:288:VAL:HG13	1.87	0.55
1:A:369:HIS:O	1:A:372:THR:HG22	2.06	0.55
1:A:188:ILE:CD1	1:A:224:ARG:HG2	2.29	0.55
1:A:447:PHE:HD1	1:A:451:ASN:HD22	1.55	0.55
1:B:16:THR:CG2	1:B:168:SER:OG	2.54	0.55
1:B:114:ASP:O	1:B:115:ASN:C	2.50	0.55
1:A:245:LYS:HE2	1:A:318:LEU:HD11	1.89	0.54
1:B:10:ILE:HG21	1:B:42:ILE:HD12	1.88	0.54
1:A:191:VAL:HG13	1:A:202:LEU:CD2	2.38	0.54
1:B:341:GLN:HG3	1:B:388:TRP:CZ2	2.42	0.54
1:B:82:PHE:CE2	1:B:502:LEU:HD23	2.42	0.54
1:B:290:CYS:SG	1:B:292:LYS:HG3	2.48	0.54
1:B:498:SER:OG	1:B:501:ALA:HB3	2.06	0.54
1:B:290:CYS:SG	1:B:292:LYS:CG	2.96	0.54
1:A:75:ILE:HG23	1:A:76:ARG:N	2.23	0.54
1:A:508:ARG:HD3	1:A:509:HIS:CD2	2.43	0.54
1:B:350:THR:HG21	1:B:391:VAL:HG11	1.89	0.53
1:B:43:GLU:O	1:B:185:SER:HA	2.09	0.53
1:B:11:ILE:HD12	1:B:41:VAL:HG22	1.90	0.53
1:B:93:LYS:HZ3	1:B:98:GLN:HB3	1.74	0.53
1:B:397:LEU:HD11	1:B:456:LEU:HD12	1.90	0.53
1:A:79:ASP:O	1:A:279:LEU:HD23	2.09	0.53
1:A:81:SER:HA	1:A:503:ILE:HD11	1.91	0.52
1:A:253:TYR:CE1	1:A:283:LYS:HG3	2.45	0.52
1:B:369:HIS:O	1:B:372:THR:HG22	2.09	0.52
1:B:464:PRO:O	1:B:465:THR:C	2.53	0.52
1:A:77:ARG:HD2	1:A:170:LEU:HD13	1.90	0.52
1:B:114:ASP:O	1:B:116:LEU:N	2.43	0.52
1:A:255:GLU:CD	1:A:258:THR:HG22	2.34	0.52
1:A:288:VAL:HG22	1:A:321:MET:CE	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:VAL:HG11	1:B:67:PHE:HA	1.90	0.52
1:B:146:THR:OG1	1:B:147:LEU:N	2.40	0.52
1:A:280:PRO:HA	1:A:500:ARG:HH12	1.75	0.52
1:B:199:ILE:CG2	1:B:215:PHE:CZ	2.92	0.52
1:B:230:MET:SD	1:B:334:CYS:HB3	2.50	0.52
1:B:370:THR:HA	1:B:373:LEU:HG	1.91	0.52
1:B:125:LYS:HG3	1:B:130:ALA:HB2	1.91	0.51
1:A:243:VAL:HG13	1:A:289:PHE:C	2.35	0.51
1:A:501:ALA:O	1:A:505:ASN:ND2	2.44	0.51
1:B:57:VAL:CG2	1:B:353:LEU:HD13	2.37	0.51
1:B:253:TYR:CE1	1:B:283:LYS:HG3	2.46	0.51
1:A:52:VAL:HG13	1:A:282:ARG:CZ	2.41	0.51
1:A:146:THR:HG22	1:A:149:CYS:SG	2.51	0.51
1:A:226:LEU:HD23	1:A:326:ARG:HD2	1.92	0.51
1:B:449:LEU:O	1:B:453:LEU:CB	2.51	0.51
1:A:448:ARG:HB3	1:A:450:GLU:CD	2.35	0.51
1:B:190:GLU:HB3	1:B:203:VAL:HB	1.93	0.51
1:A:216:ILE:HG12	1:A:335:VAL:HG13	1.91	0.51
1:B:338:GLY:O	1:B:341:GLN:HG2	2.11	0.51
1:B:396:LYS:O	1:B:397:LEU:C	2.53	0.51
1:B:93:LYS:NZ	1:B:98:GLN:HB3	2.26	0.51
1:A:448:ARG:HG3	1:A:449:LEU:H	1.76	0.51
1:B:24:HIS:CE1	1:B:360:LYS:HG3	2.46	0.51
1:B:204:ASP:CG	1:B:205:THR:N	2.69	0.51
1:B:368:THR:OG1	1:B:372:THR:HG21	2.11	0.51
1:B:26:ALA:O	1:B:27:VAL:CG2	2.54	0.50
1:A:288:VAL:CG2	1:A:321:MET:HE1	2.40	0.50
1:A:14:GLY:HA3	1:A:43:GLU:HG3	1.94	0.50
1:A:26:ALA:HB1	1:A:179:LEU:HB3	1.93	0.50
1:B:471:LEU:HD13	1:B:471:LEU:C	2.37	0.50
1:B:78:CYS:HA	1:B:166:LYS:CB	2.41	0.50
1:A:43:GLU:O	1:A:44:SER:HB3	2.12	0.50
1:A:288:VAL:CG1	1:A:321:MET:HE1	2.40	0.50
1:A:293:TYR:CE2	1:A:409:PHE:HA	2.46	0.50
1:B:464:PRO:O	1:B:466:ASN:N	2.45	0.50
1:B:235:LYS:HE2	1:B:327:GLU:HA	1.93	0.49
1:B:261:PRO:HD2	1:B:278:ALA:CB	2.42	0.49
1:A:75:ILE:HD13	1:A:506:ILE:HB	1.93	0.49
1:A:188:ILE:HD11	1:A:224:ARG:CG	2.32	0.49
1:B:240:VAL:CG1	1:B:396:LYS:HG3	2.41	0.49
1:B:365:GLN:HB3	1:B:376:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:CD2	1:A:225:LEU:HG	2.42	0.49
1:B:39:ILE:HG22	1:B:181:VAL:CG1	2.43	0.49
1:B:11:ILE:HG23	1:B:216:ILE:HB	1.93	0.49
1:B:253:TYR:HB3	1:B:258:THR:CG2	2.42	0.49
1:B:448:ARG:HE	1:B:450:GLU:CD	2.21	0.49
1:A:241:LEU:HD12	1:A:323:VAL:CG1	2.42	0.49
1:A:307:VAL:HG12	1:A:309:LYS:H	1.78	0.49
1:A:329:PHE:HE1	1:A:341:GLN:O	1.96	0.49
1:A:482:GLN:O	1:A:484:ALA:N	2.43	0.49
1:B:24:HIS:CE1	1:B:66:GLU:OE1	2.66	0.49
1:B:450:GLU:HG2	1:B:451:ASN:H	1.77	0.49
1:B:12:LEU:HD13	1:B:188:ILE:HD12	1.95	0.49
1:B:147:LEU:N	1:B:147:LEU:HD12	2.28	0.48
1:A:119:TRP:O	1:A:123:GLN:N	2.46	0.48
1:B:506:ILE:HD13	1:B:511:MET:HE2	1.95	0.48
1:A:21:THR:HG21	1:A:216:ILE:HD13	1.95	0.48
1:A:383:ARG:NH2	1:B:438:TYR:O	2.46	0.48
1:B:204:ASP:OD1	1:B:205:THR:N	2.44	0.48
1:A:75:ILE:HG23	1:A:76:ARG:HG3	1.94	0.48
1:A:142:LEU:CD1	1:A:493:MET:HB2	2.43	0.48
1:B:56:THR:HG21	1:B:60:MET:HG2	1.94	0.48
1:A:484:ALA:O	1:A:485:ILE:C	2.57	0.48
1:B:42:ILE:HG21	1:B:188:ILE:HD11	1.95	0.48
1:B:103:TYR:O	1:B:105:PRO:HD3	2.14	0.48
1:B:253:TYR:HE2	1:B:279:LEU:O	1.97	0.47
1:B:317:ARG:CZ	1:B:317:ARG:HB3	2.44	0.47
1:A:188:ILE:O	1:A:188:ILE:HG13	2.13	0.47
1:B:24:HIS:CE1	1:B:360:LYS:CG	2.97	0.47
1:A:216:ILE:HA	1:A:335:VAL:O	2.14	0.47
1:B:93:LYS:CE	1:B:99:GLU:H	2.25	0.47
1:B:10:ILE:CG2	1:B:42:ILE:HD12	2.44	0.47
1:B:341:GLN:HG3	1:B:388:TRP:HZ2	1.79	0.47
1:A:133:SER:HB3	1:A:488:ARG:HD2	1.95	0.47
1:B:77:ARG:O	1:B:79:ASP:N	2.48	0.47
1:B:468:GLN:HG2	1:B:469:LEU:N	2.28	0.47
1:B:9:VAL:HG13	1:B:39:ILE:HA	1.97	0.47
1:A:21:THR:HG21	1:A:216:ILE:HG21	1.95	0.47
1:A:38:LYS:NZ	1:A:182:GLU:OE2	2.37	0.47
1:A:80:VAL:HG22	1:A:162:LEU:HB3	1.97	0.47
1:A:347:LEU:CD2	1:A:395:ILE:HG23	2.44	0.47
1:B:21:THR:HG21	1:B:216:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:TYR:HB3	1:B:258:THR:HG21	1.96	0.47
1:A:25:LEU:CD1	1:A:29:LEU:HD11	2.45	0.47
1:A:56:THR:HG21	1:A:60:MET:HG2	1.95	0.47
1:A:130:ALA:HB1	1:A:482:GLN:HE22	1.79	0.47
1:A:38:LYS:HE3	1:A:182:GLU:OE1	2.14	0.47
1:A:12:LEU:CD2	1:A:225:LEU:CG	2.92	0.47
1:A:57:VAL:HG21	1:A:353:LEU:HD13	1.96	0.47
1:B:11:ILE:HG12	1:B:216:ILE:HG13	1.97	0.47
1:B:440:PHE:HZ	1:B:452:TYR:CG	2.33	0.47
1:A:338:GLY:HA2	1:A:355:PHE:CD1	2.50	0.46
1:B:221:PHE:CE2	1:B:322:LYS:HB2	2.49	0.46
1:A:22:ALA:HB1	1:A:181:VAL:HG11	1.98	0.46
1:A:450:GLU:HG2	1:A:451:ASN:H	1.80	0.46
1:A:27:VAL:HG11	1:A:67:PHE:HA	1.96	0.46
1:A:223:SER:O	1:A:223:SER:OG	2.30	0.46
1:A:365:GLN:HA	1:B:433:GLN:OE1	2.16	0.46
1:B:86:ILE:HG23	1:B:264:THR:O	2.15	0.46
1:A:12:LEU:CD2	1:A:225:LEU:HD11	2.39	0.46
1:A:19:TRP:CE3	1:A:172:ALA:HA	2.50	0.46
1:B:318:LEU:HD23	1:B:318:LEU:C	2.41	0.46
1:A:374:ALA:HB3	1:A:375:PRO:HD3	1.98	0.46
1:A:397:LEU:O	1:A:401:ILE:HG12	2.16	0.46
1:B:46:ASN:O	1:B:48:PRO:HD3	2.14	0.46
1:B:357:ALA:HB1	1:B:387:MET:HE1	1.97	0.46
1:A:25:LEU:HB3	1:A:39:ILE:HD11	1.97	0.46
1:A:50:ILE:HG13	1:A:52:VAL:HG23	1.97	0.46
1:A:253:TYR:HE2	1:A:279:LEU:O	1.99	0.46
1:A:347:LEU:HB3	1:A:395:ILE:HD12	1.96	0.46
1:A:347:LEU:HD22	1:A:395:ILE:HG23	1.98	0.46
1:B:115:ASN:O	1:B:118:GLN:N	2.49	0.46
1:B:136:ALA:HB1	1:B:493:MET:HE3	1.96	0.46
1:B:26:ALA:HB1	1:B:179:LEU:HB3	1.98	0.46
1:B:71:GLU:OE1	1:B:511:MET:HE1	2.16	0.46
1:A:43:GLU:O	1:A:185:SER:HA	2.15	0.45
1:A:450:GLU:HG2	1:A:451:ASN:N	2.31	0.45
1:B:115:ASN:HB3	1:B:131:PHE:CE2	2.51	0.45
1:B:14:GLY:HA3	1:B:43:GLU:OE1	2.17	0.45
1:B:311:ALA:O	1:B:313:ASP:N	2.50	0.45
1:A:137:LEU:N	1:A:137:LEU:HD12	2.31	0.45
1:A:338:GLY:C	1:A:355:PHE:CE1	2.94	0.45
1:B:112:ASP:O	1:B:113:ALA:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:TRP:CE3	1:B:172:ALA:HA	2.52	0.45
1:B:47:THR:O	1:B:47:THR:OG1	2.31	0.45
1:A:257:ASN:OD1	1:A:257:ASN:N	2.50	0.45
1:A:492:HIS:O	1:A:496:LEU:HG	2.16	0.45
1:B:270:SER:HB2	1:B:302:GLN:HE22	1.81	0.45
1:B:435:PRO:HB2	1:B:449:LEU:HD11	1.99	0.45
1:B:344:VAL:HG23	1:B:388:TRP:HZ3	1.81	0.45
1:A:338:GLY:CA	1:A:355:PHE:CE1	2.99	0.45
1:A:50:ILE:HB	1:A:165:GLY:HA3	1.99	0.45
1:B:491:HIS:O	1:B:495:GLN:HG3	2.16	0.44
1:B:155:LEU:HD11	1:B:495:GLN:OE1	2.17	0.44
1:B:24:HIS:NE2	1:B:360:LYS:HG3	2.32	0.44
1:B:194:ASP:O	1:B:196:ASP:O	2.34	0.44
1:B:374:ALA:HB3	1:B:375:PRO:HD3	2.00	0.44
1:A:449:LEU:O	1:A:453:LEU:CB	2.44	0.44
1:B:53:GLY:HA2	1:B:162:LEU:O	2.17	0.44
1:A:12:LEU:HD13	1:A:202:LEU:CD1	2.47	0.44
1:A:44:SER:O	1:A:45:PRO:C	2.61	0.44
1:A:176:GLN:HE21	1:A:183:TYR:HB2	1.83	0.44
1:B:288:VAL:CG1	1:B:321:MET:HE1	2.41	0.44
1:A:75:ILE:HD11	1:A:503:ILE:HG23	2.00	0.44
1:A:146:THR:HG23	1:A:149:CYS:H	1.82	0.44
1:B:127:PHE:O	1:B:131:PHE:HD1	2.00	0.44
1:B:350:THR:CG2	1:B:391:VAL:HG11	2.47	0.44
1:A:338:GLY:HA2	1:A:355:PHE:CZ	2.53	0.44
1:B:75:ILE:HG22	1:B:507:ILE:HD11	2.00	0.44
1:A:116:LEU:HD21	1:A:435:PRO:HD2	2.00	0.44
1:A:25:LEU:HB3	1:A:39:ILE:CD1	2.48	0.43
1:A:44:SER:H	1:A:45:PRO:HD2	1.80	0.43
1:A:328:ARG:HH12	1:A:331:HIS:CE1	2.36	0.43
1:B:240:VAL:CG1	1:B:241:LEU:CD2	2.91	0.43
1:B:260:LEU:HD22	1:B:278:ALA:HB1	2.01	0.43
1:A:92:ASN:O	1:A:93:LYS:HB2	2.19	0.43
1:A:202:LEU:HG	1:A:215:PHE:HE2	1.84	0.43
1:A:245:LYS:HE2	1:A:318:LEU:CD1	2.48	0.43
1:B:56:THR:HG1	1:B:160:TYR:H	1.61	0.43
1:B:11:ILE:HG23	1:B:216:ILE:CB	2.49	0.43
1:B:399:TYR:HB3	1:B:413:ASN:HB3	2.00	0.43
1:B:369:HIS:HE1	1:B:371:GLN:CB	2.27	0.43
1:B:499:ASN:O	1:B:503:ILE:HG13	2.18	0.43
1:A:397:LEU:HD23	1:A:455:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASP:HB3	1:A:430:TRP:CH2	2.54	0.43
1:B:166:LYS:O	1:B:169:GLU:HB2	2.19	0.43
1:B:444:PHE:O	1:B:444:PHE:CD2	2.72	0.43
1:B:221:PHE:O	1:B:222:CYS:C	2.60	0.43
1:B:108:TYR:HA	1:B:109:PRO:HD3	1.93	0.42
1:B:401:ILE:HD13	1:B:456:LEU:HA	2.00	0.42
1:B:199:ILE:HD12	1:B:230:MET:HE3	2.00	0.42
1:A:415:ASN:O	1:A:416:PRO:C	2.62	0.42
1:B:11:ILE:HA	1:B:216:ILE:HB	2.02	0.42
1:B:246:ALA:HB3	1:B:319:ILE:CG2	2.44	0.42
1:A:441:ASN:HA	1:B:443:GLY:HA3	2.01	0.42
1:B:290:CYS:SG	1:B:292:LYS:HG2	2.59	0.42
1:B:75:ILE:CD1	1:B:506:ILE:HD13	2.50	0.42
1:B:85:GLY:C	1:B:86:ILE:HG13	2.45	0.42
1:B:93:LYS:HE3	1:B:99:GLU:O	2.18	0.42
1:B:285:VAL:HG12	1:B:303:LEU:HD11	2.01	0.42
1:B:397:LEU:O	1:B:401:ILE:HG12	2.20	0.42
1:A:16:THR:HG23	1:A:167:PHE:CD2	2.55	0.42
1:A:145:LYS:HB2	1:A:145:LYS:HE3	1.31	0.42
1:A:267:THR:HG22	1:A:269:GLN:NE2	2.34	0.42
1:A:10:ILE:HG13	1:A:212:ALA:HB2	2.02	0.42
1:B:317:ARG:NH1	1:B:317:ARG:CB	2.83	0.42
1:B:133:SER:O	1:B:137:LEU:CD1	2.67	0.42
1:B:246:ALA:HA	1:B:287:HIS:O	2.20	0.42
1:A:93:LYS:NZ	1:A:99:GLU:O	2.52	0.41
1:A:137:LEU:N	1:A:137:LEU:CD1	2.83	0.41
1:B:426:ASP:HB3	1:B:430:TRP:CH2	2.55	0.41
1:A:19:TRP:HB3	1:A:171:LEU:HB3	2.02	0.41
1:A:54:GLU:CG	1:A:164:ALA:HB2	2.50	0.41
1:A:167:PHE:O	1:A:171:LEU:HG	2.20	0.41
1:B:383:ARG:O	1:B:387:MET:HG3	2.20	0.41
1:A:147:LEU:HD21	1:A:505:ASN:CG	2.45	0.41
1:A:246:ALA:HB2	1:A:321:MET:HE2	2.01	0.41
1:B:93:LYS:CE	1:B:99:GLU:O	2.68	0.41
1:A:70:SER:OG	1:A:151:GLU:CD	2.62	0.41
1:A:82:PHE:CE2	1:A:502:LEU:CD2	3.03	0.41
1:A:271:ALA:HB3	1:A:294:ILE:HD13	2.02	0.41
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.64	0.41
1:A:468:GLN:CD	1:A:468:GLN:H	2.23	0.41
1:A:202:LEU:HG	1:A:215:PHE:CE2	2.56	0.41
1:A:250:GLN:C	1:A:251:LEU:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ALA:HB1	1:B:181:VAL:HG11	2.02	0.41
1:B:254:ASP:HB2	1:B:255:GLU:OE1	2.21	0.41
1:A:191:VAL:HG13	1:A:202:LEU:HD23	2.02	0.41
1:A:389:GLU:HB3	1:A:393:ARG:NH1	2.36	0.41
1:B:82:PHE:CE2	1:B:502:LEU:CD2	3.03	0.41
1:B:225:LEU:O	1:B:229:ALA:HB3	2.20	0.41
1:B:6:ILE:HD12	1:B:373:LEU:HD21	2.02	0.41
1:B:137:LEU:HD23	1:B:496:LEU:HD13	2.03	0.41
1:A:10:ILE:HD12	1:A:215:PHE:CE2	2.56	0.41
1:A:12:LEU:CD2	1:A:225:LEU:HD21	2.47	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.93	0.41
1:A:427:LEU:HD23	1:A:430:TRP:HE3	1.85	0.41
1:A:447:PHE:HD1	1:A:451:ASN:ND2	2.18	0.41
1:A:469:LEU:HD13	1:A:469:LEU:HA	1.86	0.41
1:B:136:ALA:HB1	1:B:493:MET:HE1	2.03	0.41
1:B:103:TYR:HE2	1:B:139:ASP:OD1	2.04	0.41
1:B:230:MET:HE1	1:B:332:LYS:HB2	2.03	0.41
1:B:241:LEU:HD21	1:B:392:ILE:HG23	2.03	0.41
1:A:12:LEU:HD11	1:A:188:ILE:HG21	2.02	0.40
1:B:111:LEU:O	1:B:112:ASP:C	2.63	0.40
1:A:246:ALA:HA	1:A:287:HIS:O	2.21	0.40
1:A:307:VAL:HG12	1:A:309:LYS:HB2	2.04	0.40
1:A:427:LEU:HD23	1:A:430:TRP:CE3	2.56	0.40
1:A:482:GLN:HA	1:A:485:ILE:HG13	2.04	0.40
1:B:216:ILE:O	1:B:216:ILE:HG22	2.21	0.40
1:A:426:ASP:HB3	1:A:430:TRP:CZ3	2.57	0.40
1:B:357:ALA:CB	1:B:387:MET:HE1	2.51	0.40
1:A:14:GLY:CA	1:A:43:GLU:HG3	2.51	0.40
1:A:25:LEU:HA	1:A:25:LEU:HD13	1.85	0.40
1:B:306:TYR:CD1	1:B:306:TYR:C	2.99	0.40

All (3) 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:47:THR:CG2	1:B:311:ALA:CB[1_455]	1.69	0.51
1:B:98:GLN:NE2	1:B:182:GLU:OE1[1_565]	1.70	0.50
1:A:47:THR:CG2	1:B:312:ASN:N[1_455]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/514 (91%)	423 (90%)	43 (9%)	3 (1%)	21	53
1	B	481/514 (94%)	431 (90%)	40 (8%)	10 (2%)	5	25
All	All	950/1028 (92%)	854 (90%)	83 (9%)	13 (1%)	9	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	B	115	ASN
1	B	114	ASP
1	B	312	ASN
1	B	467	PRO
1	B	468	GLN
1	B	52	VAL
1	B	465	THR
1	B	460	ASP
1	A	52	VAL
1	A	45	PRO
1	B	34	PRO
1	B	110	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/430 (94%)	370 (92%)	33 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	412/430 (96%)	388 (94%)	24 (6%)	18	49
All	All	815/860 (95%)	758 (93%)	57 (7%)	14	42

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	49	THR
1	A	50	ILE
1	A	52	VAL
1	A	59	LEU
1	A	69	ILE
1	A	72	THR
1	A	86	ILE
1	A	93	LYS
1	A	98	GLN
1	A	99	GLU
1	A	117	THR
1	A	121	SER
1	A	123	GLN
1	A	125	LYS
1	A	145	LYS
1	A	184	LEU
1	A	194	ASP
1	A	196	ASP
1	A	226	LEU
1	A	257	ASN
1	A	279	LEU
1	A	310	GLU
1	A	326	ARG
1	A	337	ILE
1	A	345	GLU
1	A	360	LYS
1	A	391	VAL
1	A	429	HIS
1	A	467	PRO
1	A	468	GLN
1	A	485	ILE
1	A	508	ARG
1	B	6	ILE
1	B	11	ILE
1	B	33	GLN

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Mol	Chain	Res	Type
1	B	110	ILE
1	B	111	LEU
1	B	146	THR
1	B	157	SER
1	B	205	THR
1	B	208	THR
1	B	243	VAL
1	B	245	LYS
1	B	258	THR
1	B	259	VAL
1	B	274	ILE
1	B	296	THR
1	B	308	ASP
1	B	314	ILE
1	B	319	ILE
1	B	376	LEU
1	B	391	VAL
1	B	396	LYS
1	B	405	ASP
1	B	456	LEU
1	B	471	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	100	HIS
1	A	115	ASN
1	A	153	GLN
1	A	176	GLN
1	A	187	HIS
1	A	302	GLN
1	A	365	GLN
1	A	415	ASN
1	A	433	GLN
1	A	451	ASN
1	A	466	ASN
1	A	495	GLN
1	A	509	HIS
1	B	24	HIS
1	B	62	HIS
1	B	176	GLN

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Mol	Chain	Res	Type
1	B	178	ASN
1	B	300	HIS
1	B	302	GLN
1	B	365	GLN
1	B	369	HIS
1	B	403	ASN
1	B	429	HIS
1	B	442	GLN
1	B	491	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	483/514 (93%)	2.13	239 (49%) 0 0	35, 46, 61, 74	0
1	B	493/514 (95%)	2.21	252 (51%) 0 0	30, 46, 63, 78	0
All	All	976/1028 (94%)	2.17	491 (50%) 0 0	30, 46, 63, 78	0

All (491) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	ALA	8.5
1	A	462	ALA	6.8
1	A	147	LEU	6.7
1	A	309	LYS	6.5
1	B	50	ILE	6.1
1	B	402	SER	6.1
1	B	375	PRO	5.6
1	B	444	PHE	5.6
1	B	514	VAL	5.5
1	B	471	LEU	5.4
1	B	6	ILE	5.4
1	A	470	ALA	5.3
1	A	188	ILE	5.3
1	A	308	ASP	5.3
1	B	98	GLN	5.2
1	B	10	ILE	5.2
1	B	112	ASP	5.1
1	B	216	ILE	5.1
1	B	182	GLU	5.0
1	A	90	ALA	5.0
1	A	45	PRO	5.0
1	B	469	LEU	5.0
1	A	319	ILE	4.9
1	B	239	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	418	SER	4.8
1	A	293	TYR	4.8
1	B	93	LYS	4.7
1	B	464	PRO	4.7
1	B	486	ALA	4.7
1	B	446	THR	4.7
1	A	228	GLU	4.6
1	A	254	ASP	4.5
1	B	197	GLY	4.5
1	B	113	ALA	4.5
1	B	92	ASN	4.5
1	B	45	PRO	4.5
1	B	466	ASN	4.5
1	A	297	ASP	4.4
1	A	42	ILE	4.4
1	B	15	GLY	4.4
1	A	469	LEU	4.4
1	A	406	ASP	4.4
1	B	69	ILE	4.4
1	A	52	VAL	4.4
1	A	256	PRO	4.4
1	A	299	ALA	4.3
1	B	467	PRO	4.3
1	B	44	SER	4.3
1	B	111	LEU	4.3
1	A	248	ALA	4.3
1	A	486	ALA	4.3
1	A	75	ILE	4.3
1	B	322	LYS	4.3
1	A	347	LEU	4.3
1	A	361	LEU	4.3
1	B	62	HIS	4.2
1	A	301	ALA	4.2
1	B	507	ILE	4.2
1	A	12	LEU	4.2
1	A	468	GLN	4.1
1	A	311	ALA	4.1
1	B	208	THR	4.0
1	B	30	LYS	4.0
1	A	310	GLU	4.0
1	A	4	HIS	4.0
1	A	242	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	241	LEU	4.0
1	A	129	HIS	4.0
1	A	359	ALA	3.9
1	B	73	ASP	3.9
1	A	322	LYS	3.9
1	B	34	PRO	3.9
1	A	401	ILE	3.9
1	A	464	PRO	3.9
1	B	110	ILE	3.9
1	B	392	ILE	3.9
1	B	305	SER	3.9
1	A	443	GLY	3.9
1	B	259	VAL	3.9
1	A	408	ASP	3.8
1	B	89	ASN	3.8
1	B	238	SER	3.8
1	A	49	THR	3.8
1	A	342	GLY	3.8
1	B	416	PRO	3.8
1	B	52	VAL	3.7
1	A	50	ILE	3.7
1	A	216	ILE	3.7
1	A	115	ASN	3.7
1	B	403	ASN	3.7
1	B	51	GLY	3.7
1	B	313	ASP	3.7
1	B	417	ALA	3.7
1	A	48	PRO	3.7
1	B	455	VAL	3.7
1	A	362	LEU	3.6
1	B	200	SER	3.6
1	A	14	GLY	3.6
1	A	291	ASP	3.6
1	A	44	SER	3.6
1	A	377	ALA	3.6
1	A	412	ASP	3.6
1	B	210	TYR	3.6
1	B	465	THR	3.6
1	B	274	ILE	3.5
1	A	388	TRP	3.5
1	B	205	THR	3.5
1	A	19	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	403	ASN	3.5
1	A	243	VAL	3.5
1	B	224	ARG	3.5
1	A	21	THR	3.5
1	A	222	CYS	3.5
1	B	369	HIS	3.5
1	B	399	TYR	3.5
1	A	466	ASN	3.5
1	B	453	LEU	3.4
1	B	270	SER	3.4
1	A	244	ASN	3.4
1	B	371	GLN	3.4
1	B	425	ASN	3.4
1	A	321	MET	3.4
1	A	449	LEU	3.4
1	B	263	CYS	3.4
1	A	467	PRO	3.4
1	B	101	SER	3.4
1	A	56	THR	3.4
1	A	320	ASP	3.4
1	A	405	ASP	3.4
1	B	449	LEU	3.4
1	A	507	ILE	3.4
1	A	343	PHE	3.4
1	B	35	GLY	3.4
1	B	211	LYS	3.4
1	A	46	ASN	3.3
1	A	271	ALA	3.3
1	A	273	TRP	3.3
1	A	337	ILE	3.3
1	B	377	ALA	3.3
1	A	134	GLN	3.3
1	A	409	PHE	3.3
1	B	293	TYR	3.3
1	B	386	GLY	3.3
1	A	259	VAL	3.3
1	A	108	TYR	3.3
1	B	314	ILE	3.3
1	A	249	LEU	3.3
1	B	468	GLN	3.3
1	B	40	THR	3.3
1	A	15	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	169	GLU	3.2
1	B	406	ASP	3.2
1	A	375	PRO	3.2
1	B	493	MET	3.2
1	A	118	GLN	3.2
1	A	365	GLN	3.2
1	B	41	VAL	3.2
1	B	85	GLY	3.2
1	A	158	TYR	3.2
1	A	31	PRO	3.2
1	A	230	MET	3.2
1	B	188	ILE	3.2
1	A	400	ALA	3.2
1	B	179	LEU	3.2
1	B	391	VAL	3.2
1	B	64	LEU	3.2
1	B	141	ALA	3.2
1	B	422	ALA	3.2
1	B	146	THR	3.2
1	B	117	THR	3.2
1	B	388	TRP	3.2
1	A	312	ASN	3.1
1	A	57	VAL	3.1
1	B	243	VAL	3.1
1	A	193	LEU	3.1
1	B	273	TRP	3.1
1	A	340	ALA	3.1
1	B	135	ALA	3.1
1	B	310	GLU	3.1
1	B	376	LEU	3.1
1	A	102	TYR	3.1
1	B	129	HIS	3.1
1	A	402	SER	3.1
1	A	363	ALA	3.0
1	B	136	ALA	3.0
1	A	432	HIS	3.0
1	B	275	TRP	3.0
1	A	510	GLY	3.0
1	B	353	LEU	3.0
1	A	422	ALA	3.0
1	B	501	ALA	3.0
1	B	410	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	77	ARG	3.0
1	B	424	LYS	3.0
1	B	162	LEU	3.0
1	A	117	THR	3.0
1	B	359	ALA	3.0
1	B	307	VAL	3.0
1	A	168	SER	3.0
1	B	59	LEU	3.0
1	B	421	GLU	3.0
1	B	330	TRP	3.0
1	A	260	LEU	3.0
1	B	53	GLY	3.0
1	B	269	GLN	3.0
1	B	295	SER	3.0
1	A	444	PHE	3.0
1	B	203	VAL	3.0
1	A	369	HIS	2.9
1	A	171	LEU	2.9
1	A	416	PRO	2.9
1	B	315	ALA	2.9
1	B	335	VAL	2.9
1	B	16	THR	2.9
1	B	56	THR	2.9
1	B	225	LEU	2.9
1	A	302	GLN	2.9
1	B	327	GLU	2.9
1	B	196	ASP	2.9
1	B	445	ASP	2.9
1	B	128	SER	2.9
1	B	447	PHE	2.9
1	B	491	HIS	2.9
1	B	362	LEU	2.9
1	A	275	TRP	2.9
1	B	316	PRO	2.9
1	B	195	ASP	2.9
1	A	264	THR	2.9
1	B	277	ILE	2.9
1	A	13	GLY	2.8
1	A	98	GLN	2.8
1	B	452	TYR	2.8
1	B	502	LEU	2.8
1	A	51	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	438	TYR	2.8
1	A	135	ALA	2.8
1	B	462	ALA	2.8
1	A	413	ASN	2.8
1	B	337	ILE	2.8
1	B	230	MET	2.8
1	A	292	LYS	2.8
1	A	269	GLN	2.8
1	A	169	GLU	2.8
1	A	190	GLU	2.8
1	A	298	GLU	2.8
1	B	271	ALA	2.8
1	B	343	PHE	2.8
1	B	321	MET	2.8
1	B	308	ASP	2.8
1	B	226	LEU	2.7
1	B	395	ILE	2.7
1	B	506	ILE	2.7
1	A	187	HIS	2.7
1	B	49	THR	2.7
1	B	296	THR	2.7
1	A	318	LEU	2.7
1	A	366	PHE	2.7
1	A	300	HIS	2.7
1	B	309	LYS	2.7
1	A	346	PRO	2.7
1	B	504	GLU	2.7
1	B	240	VAL	2.7
1	B	106	PHE	2.7
1	B	304	ALA	2.7
1	B	4	HIS	2.7
1	B	194	ASP	2.7
1	A	143	ALA	2.7
1	A	324	GLY	2.7
1	B	13	GLY	2.7
1	A	433	GLN	2.7
1	A	6	ILE	2.6
1	A	353	LEU	2.7
1	B	12	LEU	2.7
1	A	372	THR	2.6
1	B	147	LEU	2.6
1	A	294	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	392	ILE	2.6
1	B	319	ILE	2.6
1	A	270	SER	2.6
1	A	303	LEU	2.6
1	B	298	GLU	2.6
1	A	262	SER	2.6
1	B	209	HIS	2.6
1	A	91	TRP	2.6
1	A	306	TYR	2.6
1	A	261	PRO	2.6
1	B	126	PRO	2.6
1	A	263	CYS	2.6
1	A	208	THR	2.6
1	A	296	THR	2.6
1	A	92	ASN	2.6
1	A	172	ALA	2.6
1	A	330	TRP	2.6
1	B	456	LEU	2.6
1	A	285	VAL	2.6
1	A	465	THR	2.6
1	B	264	THR	2.6
1	A	136	ALA	2.6
1	A	440	PHE	2.6
1	B	483	ASP	2.6
1	A	121	SER	2.5
1	B	223	SER	2.5
1	A	97	GLY	2.5
1	B	247	LEU	2.5
1	B	352	LEU	2.5
1	A	240	VAL	2.5
1	B	72	THR	2.5
1	B	440	PHE	2.5
1	B	451	ASN	2.5
1	A	225	LEU	2.5
1	B	251	LEU	2.5
1	B	183	TYR	2.5
1	B	311	ALA	2.5
1	A	161	HIS	2.5
1	A	245	LYS	2.5
1	A	101	SER	2.5
1	B	361	LEU	2.5
1	A	277	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	103	TYR	2.5
1	B	108	TYR	2.5
1	A	67	PHE	2.5
1	B	61	ALA	2.5
1	B	290	CYS	2.5
1	A	395	ILE	2.5
1	B	14	GLY	2.5
1	B	233	GLY	2.5
1	A	181	VAL	2.5
1	A	380	PHE	2.5
1	A	452	TYR	2.5
1	B	215	PHE	2.5
1	B	394	PHE	2.5
1	A	276	ASP	2.4
1	B	20	LEU	2.4
1	B	60	MET	2.4
1	B	58	PRO	2.4
1	B	86	ILE	2.4
1	B	323	VAL	2.4
1	A	145	LYS	2.4
1	A	153	GLN	2.4
1	A	357	ALA	2.4
1	A	139	ASP	2.4
1	A	344	VAL	2.4
1	B	99	GLU	2.4
1	B	127	PHE	2.4
1	A	371	GLN	2.4
1	B	193	LEU	2.4
1	A	35	GLY	2.4
1	B	114	ASP	2.4
1	B	385	SER	2.4
1	B	409	PHE	2.4
1	A	246	ALA	2.4
1	B	341	GLN	2.4
1	B	368	THR	2.4
1	A	352	LEU	2.4
1	B	48	PRO	2.4
1	B	366	PHE	2.4
1	B	336	ALA	2.4
1	B	374	ALA	2.4
1	B	168	SER	2.4
1	A	251	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	453	LEU	2.4
1	B	184	LEU	2.4
1	A	10	ILE	2.4
1	A	34	PRO	2.4
1	A	93	LYS	2.3
1	A	393	ARG	2.3
1	B	283	LYS	2.3
1	B	357	ALA	2.3
1	A	162	LEU	2.3
1	A	339	LEU	2.3
1	B	25	LEU	2.3
1	A	500	ARG	2.3
1	A	159	GLY	2.3
1	B	365	GLN	2.3
1	A	132	SER	2.3
1	B	303	LEU	2.3
1	B	397	LEU	2.3
1	B	191	VAL	2.3
1	B	232	VAL	2.3
1	B	338	GLY	2.3
1	A	257	ASN	2.3
1	A	505	ASN	2.3
1	B	124	ASP	2.3
1	A	471	LEU	2.3
1	A	429	HIS	2.3
1	B	91	TRP	2.3
1	B	509	HIS	2.3
1	A	128	SER	2.3
1	A	488	ARG	2.3
1	B	306	TYR	2.3
1	A	272	GLY	2.3
1	B	329	PHE	2.3
1	A	26	ALA	2.3
1	A	186	ALA	2.3
1	A	417	ALA	2.3
1	B	301	ALA	2.3
1	A	334	CYS	2.3
1	B	294	ILE	2.3
1	A	512	SER	2.3
1	A	289	PHE	2.2
1	A	226	LEU	2.2
1	B	411	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	404	ARG	2.2
1	B	119	TRP	2.2
1	B	8	SER	2.2
1	A	54	GLU	2.2
1	A	116	LEU	2.2
1	A	345	GLU	2.2
1	B	29	LEU	2.2
1	B	415	ASN	2.2
1	B	161	HIS	2.2
1	B	492	HIS	2.2
1	A	9	VAL	2.2
1	A	410	TRP	2.2
1	B	19	TRP	2.2
1	A	351	GLY	2.2
1	B	234	PHE	2.2
1	A	22	ALA	2.2
1	B	265	LEU	2.2
1	B	503	ILE	2.2
1	B	460	ASP	2.2
1	B	261	PRO	2.2
1	A	368	THR	2.2
1	B	350	THR	2.2
1	B	116	LEU	2.2
1	A	229	ALA	2.2
1	B	11	ILE	2.2
1	A	209	HIS	2.2
1	A	492	HIS	2.2
1	A	509	HIS	2.2
1	B	204	ASP	2.2
1	A	253	TYR	2.2
1	B	481	LEU	2.2
1	B	43	GLU	2.2
1	A	250	GLN	2.1
1	A	415	ASN	2.1
1	B	432	HIS	2.1
1	A	493	MET	2.1
1	B	163	ASP	2.1
1	B	258	THR	2.1
1	A	167	PHE	2.1
1	A	221	PHE	2.1
1	A	430	TRP	2.1
1	B	380	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	438	TYR	2.1
1	A	290	CYS	2.1
1	A	495	GLN	2.1
1	B	104	HIS	2.1
1	A	79	ASP	2.1
1	B	165	GLY	2.1
1	B	324	GLY	2.1
1	A	461	PHE	2.1
1	A	354	VAL	2.1
1	A	445	ASP	2.1
1	B	242	PHE	2.1
1	B	461	PHE	2.1
1	A	84	GLN	2.1
1	A	307	VAL	2.1
1	A	265	LEU	2.1
1	A	356	ASP	2.1
1	A	446	THR	2.1
1	A	39	ILE	2.1
1	A	86	ILE	2.1
1	A	122	ALA	2.1
1	A	304	ALA	2.1
1	A	255	GLU	2.1
1	A	399	TYR	2.1
1	B	457	TYR	2.1
1	B	396	LYS	2.0
1	B	512	SER	2.0
1	B	5	PRO	2.0
1	B	23	ASN	2.0
1	A	76	ARG	2.0
1	B	74	PHE	2.0
1	B	443	GLY	2.0
1	B	246	ALA	2.0
1	A	152	TYR	2.0
1	A	41	VAL	2.0
1	A	185	SER	2.0
1	A	232	VAL	2.0
1	A	287	HIS	2.0
1	A	418	SER	2.0
1	A	498	SER	2.0
1	B	344	VAL	2.0
1	B	180	GLY	2.0
1	A	274	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	42	ILE	2.0
1	A	349	ALA	2.0
1	B	186	ALA	2.0
1	B	400	ALA	2.0
1	B	57	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.