



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:06 AM UTC

PDB ID : 5XRC / pdb_00005xrc
Title : A Trimodular GH5_4 Subfamily Endoglucanase Structure with Large Unit Cell
Authors : Zhang, H.D.
Deposited on : 2017-06-08
Resolution : 2.90 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

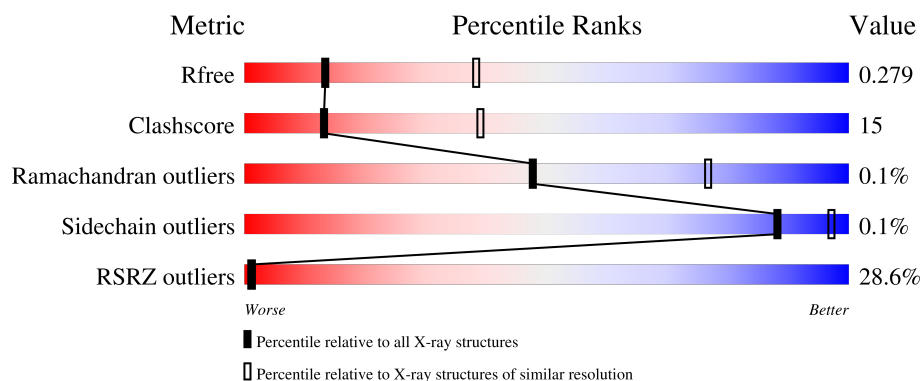
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	585	4% 71% 20% 9%
1	B	585	71% 54% 36% 9%
1	C	585	3% 69% 21% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12970 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 Cellulase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4312	2724	727	848	13			
1	B	530	Total	C	N	O	S	0	0	0
			4303	2719	725	846	13			
1	C	532	Total	C	N	O	S	0	0	0
			4321	2730	729	849	13			

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP D4P8C6
A	-32	GLY	-	expression tag	UNP D4P8C6
A	-31	SER	-	expression tag	UNP D4P8C6
A	-30	SER	-	expression tag	UNP D4P8C6
A	-29	HIS	-	expression tag	UNP D4P8C6
A	-28	HIS	-	expression tag	UNP D4P8C6
A	-27	HIS	-	expression tag	UNP D4P8C6
A	-26	HIS	-	expression tag	UNP D4P8C6
A	-25	HIS	-	expression tag	UNP D4P8C6
A	-24	HIS	-	expression tag	UNP D4P8C6
A	-23	SER	-	expression tag	UNP D4P8C6
A	-22	SER	-	expression tag	UNP D4P8C6
A	-21	GLY	-	expression tag	UNP D4P8C6
A	-20	LEU	-	expression tag	UNP D4P8C6
A	-19	VAL	-	expression tag	UNP D4P8C6
A	-18	PRO	-	expression tag	UNP D4P8C6
A	-17	ARG	-	expression tag	UNP D4P8C6
A	-16	GLY	-	expression tag	UNP D4P8C6
A	-15	SER	-	expression tag	UNP D4P8C6
A	-14	HIS	-	expression tag	UNP D4P8C6
A	-13	MET	-	expression tag	UNP D4P8C6
A	-12	ALA	-	expression tag	UNP D4P8C6
A	-11	SER	-	expression tag	UNP D4P8C6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP D4P8C6
A	-9	THR	-	expression tag	UNP D4P8C6
A	-8	GLY	-	expression tag	UNP D4P8C6
A	-7	GLY	-	expression tag	UNP D4P8C6
A	-6	GLN	-	expression tag	UNP D4P8C6
A	-5	GLN	-	expression tag	UNP D4P8C6
A	-4	MET	-	expression tag	UNP D4P8C6
A	-3	GLY	-	expression tag	UNP D4P8C6
A	-2	ARG	-	expression tag	UNP D4P8C6
A	-1	GLY	-	expression tag	UNP D4P8C6
A	0	SER	-	expression tag	UNP D4P8C6
A	537	VAL	-	expression tag	UNP D4P8C6
A	538	ASP	-	expression tag	UNP D4P8C6
A	539	LYS	-	expression tag	UNP D4P8C6
A	540	LEU	-	expression tag	UNP D4P8C6
A	541	ALA	-	expression tag	UNP D4P8C6
A	542	ALA	-	expression tag	UNP D4P8C6
A	543	ALA	-	expression tag	UNP D4P8C6
A	544	LEU	-	expression tag	UNP D4P8C6
A	545	GLU	-	expression tag	UNP D4P8C6
A	546	HIS	-	expression tag	UNP D4P8C6
A	547	HIS	-	expression tag	UNP D4P8C6
A	548	HIS	-	expression tag	UNP D4P8C6
A	549	HIS	-	expression tag	UNP D4P8C6
A	550	HIS	-	expression tag	UNP D4P8C6
A	551	HIS	-	expression tag	UNP D4P8C6
B	-33	MET	-	expression tag	UNP D4P8C6
B	-32	GLY	-	expression tag	UNP D4P8C6
B	-31	SER	-	expression tag	UNP D4P8C6
B	-30	SER	-	expression tag	UNP D4P8C6
B	-29	HIS	-	expression tag	UNP D4P8C6
B	-28	HIS	-	expression tag	UNP D4P8C6
B	-27	HIS	-	expression tag	UNP D4P8C6
B	-26	HIS	-	expression tag	UNP D4P8C6
B	-25	HIS	-	expression tag	UNP D4P8C6
B	-24	HIS	-	expression tag	UNP D4P8C6
B	-23	SER	-	expression tag	UNP D4P8C6
B	-22	SER	-	expression tag	UNP D4P8C6
B	-21	GLY	-	expression tag	UNP D4P8C6
B	-20	LEU	-	expression tag	UNP D4P8C6
B	-19	VAL	-	expression tag	UNP D4P8C6
B	-18	PRO	-	expression tag	UNP D4P8C6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	ARG	-	expression tag	UNP D4P8C6
B	-16	GLY	-	expression tag	UNP D4P8C6
B	-15	SER	-	expression tag	UNP D4P8C6
B	-14	HIS	-	expression tag	UNP D4P8C6
B	-13	MET	-	expression tag	UNP D4P8C6
B	-12	ALA	-	expression tag	UNP D4P8C6
B	-11	SER	-	expression tag	UNP D4P8C6
B	-10	MET	-	expression tag	UNP D4P8C6
B	-9	THR	-	expression tag	UNP D4P8C6
B	-8	GLY	-	expression tag	UNP D4P8C6
B	-7	GLY	-	expression tag	UNP D4P8C6
B	-6	GLN	-	expression tag	UNP D4P8C6
B	-5	GLN	-	expression tag	UNP D4P8C6
B	-4	MET	-	expression tag	UNP D4P8C6
B	-3	GLY	-	expression tag	UNP D4P8C6
B	-2	ARG	-	expression tag	UNP D4P8C6
B	-1	GLY	-	expression tag	UNP D4P8C6
B	0	SER	-	expression tag	UNP D4P8C6
B	537	VAL	-	expression tag	UNP D4P8C6
B	538	ASP	-	expression tag	UNP D4P8C6
B	539	LYS	-	expression tag	UNP D4P8C6
B	540	LEU	-	expression tag	UNP D4P8C6
B	541	ALA	-	expression tag	UNP D4P8C6
B	542	ALA	-	expression tag	UNP D4P8C6
B	543	ALA	-	expression tag	UNP D4P8C6
B	544	LEU	-	expression tag	UNP D4P8C6
B	545	GLU	-	expression tag	UNP D4P8C6
B	546	HIS	-	expression tag	UNP D4P8C6
B	547	HIS	-	expression tag	UNP D4P8C6
B	548	HIS	-	expression tag	UNP D4P8C6
B	549	HIS	-	expression tag	UNP D4P8C6
B	550	HIS	-	expression tag	UNP D4P8C6
B	551	HIS	-	expression tag	UNP D4P8C6
C	-33	MET	-	expression tag	UNP D4P8C6
C	-32	GLY	-	expression tag	UNP D4P8C6
C	-31	SER	-	expression tag	UNP D4P8C6
C	-30	SER	-	expression tag	UNP D4P8C6
C	-29	HIS	-	expression tag	UNP D4P8C6
C	-28	HIS	-	expression tag	UNP D4P8C6
C	-27	HIS	-	expression tag	UNP D4P8C6
C	-26	HIS	-	expression tag	UNP D4P8C6
C	-25	HIS	-	expression tag	UNP D4P8C6

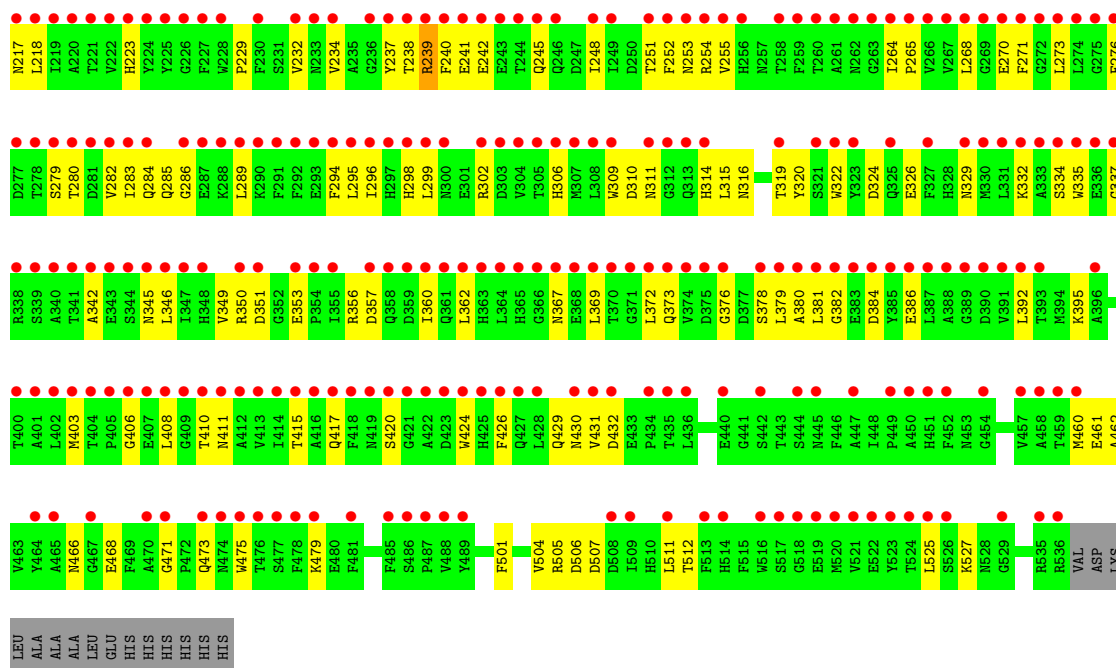
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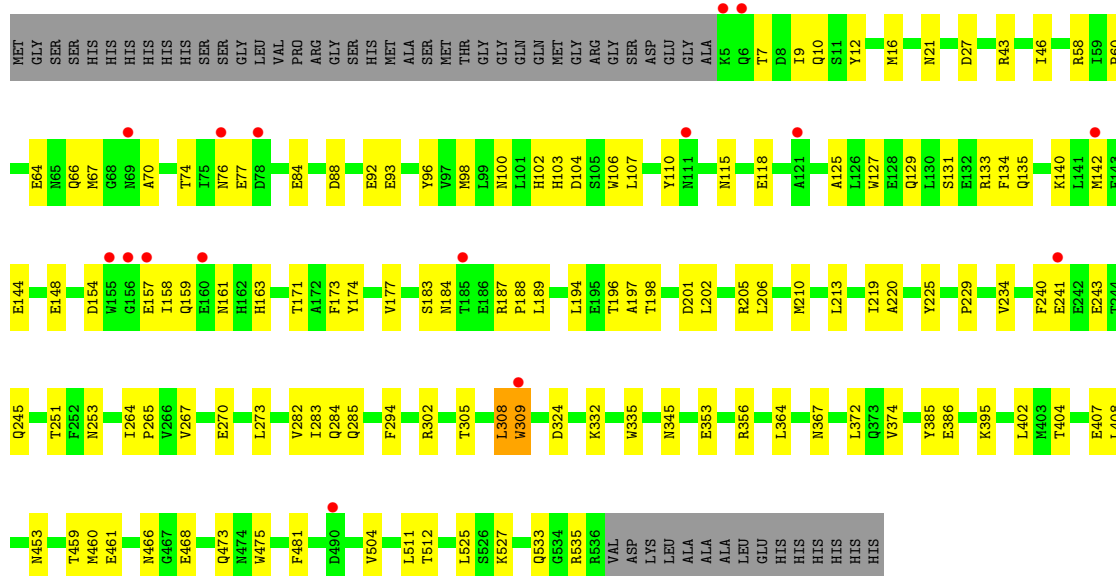
Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	HIS	-	expression tag	UNP D4P8C6
C	-23	SER	-	expression tag	UNP D4P8C6
C	-22	SER	-	expression tag	UNP D4P8C6
C	-21	GLY	-	expression tag	UNP D4P8C6
C	-20	LEU	-	expression tag	UNP D4P8C6
C	-19	VAL	-	expression tag	UNP D4P8C6
C	-18	PRO	-	expression tag	UNP D4P8C6
C	-17	ARG	-	expression tag	UNP D4P8C6
C	-16	GLY	-	expression tag	UNP D4P8C6
C	-15	SER	-	expression tag	UNP D4P8C6
C	-14	HIS	-	expression tag	UNP D4P8C6
C	-13	MET	-	expression tag	UNP D4P8C6
C	-12	ALA	-	expression tag	UNP D4P8C6
C	-11	SER	-	expression tag	UNP D4P8C6
C	-10	MET	-	expression tag	UNP D4P8C6
C	-9	THR	-	expression tag	UNP D4P8C6
C	-8	GLY	-	expression tag	UNP D4P8C6
C	-7	GLY	-	expression tag	UNP D4P8C6
C	-6	GLN	-	expression tag	UNP D4P8C6
C	-5	GLN	-	expression tag	UNP D4P8C6
C	-4	MET	-	expression tag	UNP D4P8C6
C	-3	GLY	-	expression tag	UNP D4P8C6
C	-2	ARG	-	expression tag	UNP D4P8C6
C	-1	GLY	-	expression tag	UNP D4P8C6
C	0	SER	-	expression tag	UNP D4P8C6
C	537	VAL	-	expression tag	UNP D4P8C6
C	538	ASP	-	expression tag	UNP D4P8C6
C	539	LYS	-	expression tag	UNP D4P8C6
C	540	LEU	-	expression tag	UNP D4P8C6
C	541	ALA	-	expression tag	UNP D4P8C6
C	542	ALA	-	expression tag	UNP D4P8C6
C	543	ALA	-	expression tag	UNP D4P8C6
C	544	LEU	-	expression tag	UNP D4P8C6
C	545	GLU	-	expression tag	UNP D4P8C6
C	546	HIS	-	expression tag	UNP D4P8C6
C	547	HIS	-	expression tag	UNP D4P8C6
C	548	HIS	-	expression tag	UNP D4P8C6
C	549	HIS	-	expression tag	UNP D4P8C6
C	550	HIS	-	expression tag	UNP D4P8C6
C	551	HIS	-	expression tag	UNP D4P8C6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total 8	O 8	0	0
2	B	1	Total 1	O 1	0	0
2	C	25	Total 25	O 25	0	0



● Molecule 1: Cellulase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.14Å 120.14Å 615.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.97 – 2.90 85.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (85.97-2.90) 99.0 (85.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.276 , 0.332 (Not available) , 0.279	Depositor DCC
R_{free} test set	2408 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12970	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9383e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.22	1/4430 (0.0%)	0.47	4/6032 (0.1%)
1	B	0.29	0/4421	0.63	8/6020 (0.1%)
1	C	0.26	1/4439 (0.0%)	0.49	6/6043 (0.1%)
All	All	0.26	2/13290 (0.0%)	0.54	18/18095 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	308	LEU	C-N	-13.78	1.13	1.33
1	A	211	LYS	CG-CD	5.37	1.68	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	309	TRP	O-C-N	13.58	138.70	123.22
1	A	211	LYS	CA-CB-CG	7.91	129.93	114.10
1	B	239	ARG	CG-CD-NE	-7.16	96.25	112.00
1	C	308	LEU	CA-C-N	7.15	132.28	122.77
1	C	308	LEU	C-N-CA	7.15	132.28	122.77
1	B	186	GLU	CB-CG-CD	7.08	124.64	112.60
1	C	308	LEU	O-C-N	-6.67	115.00	122.86
1	C	309	TRP	CA-C-N	-6.50	113.60	122.95
1	C	309	TRP	C-N-CA	-6.50	113.60	122.95
1	A	318	GLU	CA-CB-CG	6.11	126.31	114.10
1	B	159	GLN	CA-C-N	6.07	133.14	121.54
1	B	159	GLN	C-N-CA	6.07	133.14	121.54
1	B	239	ARG	CA-CB-CG	6.00	126.09	114.10
1	A	318	GLU	CB-CA-C	5.98	118.61	109.34
1	A	211	LYS	CB-CA-C	-5.85	101.08	110.79
1	B	186	GLU	CA-CB-CG	5.13	124.36	114.10
1	B	238	THR	CA-C-N	5.05	131.93	121.32
1	B	238	THR	C-N-CA	5.05	131.93	121.32

There are no chirality outliers.

There are no planarity outliers.

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	4312	0	3976	90	0
1	B	4303	0	3968	195	0
1	C	4321	0	3988	87	0
2	A	8	0	0	1	0
2	B	1	0	0	0	0
2	C	25	0	0	0	0
All	All	12970	0	11932	370	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 15.

All (370) 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:379:LEU:HD21	1:B:384:ASP:CG	1.51	1.35
1:B:360:ILE:HD11	1:B:426:PHE:CE2	1.69	1.28
1:B:424:TRP:CD1	1:B:426:PHE:CE1	2.20	1.27
1:B:379:LEU:HD21	1:B:384:ASP:OD2	1.09	1.19
1:B:381:LEU:HD23	1:B:382:GLY:N	1.57	1.17
1:B:379:LEU:HD23	1:B:380:ALA:N	1.60	1.17
1:B:379:LEU:CD2	1:B:384:ASP:OD2	1.92	1.16
1:B:379:LEU:HD21	1:B:384:ASP:CB	1.83	1.09
1:B:424:TRP:CD1	1:B:426:PHE:HE1	1.65	1.07
1:B:379:LEU:CD2	1:B:384:ASP:CB	2.41	0.98
1:B:379:LEU:CD2	1:B:384:ASP:HB2	1.94	0.97
1:B:424:TRP:NE1	1:B:426:PHE:CE1	2.34	0.95
1:B:360:ILE:HD11	1:B:426:PHE:HE2	1.28	0.94
1:B:91:LEU:HD21	1:B:97:VAL:HG23	1.52	0.92
1:B:268:LEU:HD21	1:B:271:PHE:HB3	1.53	0.91
1:B:424:TRP:HD1	1:B:426:PHE:CE1	1.91	0.89
1:B:424:TRP:CD1	1:B:426:PHE:CD1	2.61	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:GLU:OE1	1:C:356:ARG:NH2	2.07	0.87
1:A:207:HIS:CE1	1:A:211:LYS:HE2	2.11	0.86
1:B:276:PHE:HD1	1:B:280:THR:HA	1.39	0.84
1:B:381:LEU:HD23	1:B:382:GLY:H	1.41	0.83
1:B:379:LEU:HD22	1:B:384:ASP:HB2	1.59	0.82
1:C:171:THR:HG22	1:C:213:LEU:HD11	1.62	0.81
1:A:370:THR:O	2:A:601:HOH:O	1.98	0.80
1:B:27:ASP:HB2	1:B:102:HIS:CD2	2.16	0.79
1:A:207:HIS:CE1	1:A:211:LYS:CE	2.66	0.79
1:B:329:ASN:HA	1:B:332:LYS:NZ	1.99	0.78
1:B:42:THR:HG22	1:B:44:GLU:H	1.46	0.78
1:B:296:ILE:HA	1:B:299:LEU:HD12	1.67	0.75
1:B:424:TRP:HD1	1:B:426:PHE:CD1	2.00	0.74
1:A:229:PRO:HB2	1:A:237:TYR:HD2	1.52	0.74
1:B:273:LEU:HB2	1:B:276:PHE:CE2	2.22	0.74
1:A:154:ASP:HB2	1:A:155:TRP:HE3	1.52	0.74
1:B:13:VAL:HA	1:B:16:MET:HE3	1.68	0.74
1:A:154:ASP:HB2	1:A:155:TRP:CE3	2.23	0.73
1:A:437:GLU:HB2	1:A:449:PRO:HG2	1.71	0.73
1:B:151:PHE:HB2	1:B:162:HIS:CD2	2.24	0.73
1:B:23:GLY:HA3	1:B:309:TRP:CZ3	2.24	0.72
1:B:159:GLN:HG2	1:B:162:HIS:ND1	2.04	0.72
1:B:218:LEU:O	1:B:264:ILE:HD11	1.90	0.72
1:C:66:GLN:OE1	1:C:76:ASN:ND2	2.23	0.72
1:A:440:GLU:OE2	1:A:533:GLN:NE2	2.23	0.72
1:B:342:ALA:CB	1:B:426:PHE:HZ	2.04	0.71
1:C:210:MET:HE1	1:C:220:ALA:HB2	1.72	0.70
1:B:298:HIS:O	1:B:302:ARG:HD2	1.91	0.70
1:A:264:ILE:HD12	1:A:265:PRO:HD2	1.73	0.70
1:B:360:ILE:HD11	1:B:426:PHE:CD2	2.27	0.69
1:C:74:THR:HA	1:C:129:GLN:HE22	1.58	0.68
1:B:309:TRP:CZ2	1:B:311:ASN:HB3	2.29	0.68
1:C:58:ARG:NH2	1:C:270:GLU:OE2	2.26	0.68
1:B:46:ILE:HD11	1:B:89:TRP:HB3	1.76	0.68
1:A:190:VAL:HG12	1:A:221:THR:OG1	1.94	0.68
1:B:147:ASN:OD1	1:B:148:GLU:HG3	1.95	0.67
1:B:379:LEU:HD23	1:B:380:ALA:H	1.56	0.66
1:B:379:LEU:HD23	1:B:379:LEU:C	2.19	0.66
1:B:329:ASN:HA	1:B:332:LYS:HZ2	1.60	0.66
1:B:373:GLN:OE1	1:B:376:GLY:HA2	1.94	0.66
1:C:253:ASN:HD21	1:C:302:ARG:HH21	1.40	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:PRO:HB2	1:A:237:TYR:CD2	2.31	0.65
1:B:174:TYR:HD2	1:B:213:LEU:HD22	1.62	0.65
1:B:276:PHE:CD1	1:B:280:THR:HA	2.27	0.65
1:B:410:THR:OG1	1:B:429:GLN:NE2	2.25	0.64
1:B:360:ILE:CD1	1:B:426:PHE:CE2	2.64	0.64
1:B:460:MET:HE2	1:B:479:LYS:HG3	1.79	0.64
1:C:7:THR:HG22	1:C:9:ILE:H	1.63	0.64
1:B:284:GLN:OE1	1:B:285:GLN:N	2.30	0.64
1:C:16:MET:HB2	1:C:305:THR:HG21	1.80	0.64
1:C:184:ASN:OD1	1:C:187:ARG:NH1	2.30	0.63
1:B:253:ASN:OD1	1:B:302:ARG:NH1	2.28	0.63
1:B:31:ASP:O	1:B:66:GLN:NE2	2.31	0.63
1:B:89:TRP:HA	1:B:92:GLU:HG3	1.80	0.62
1:C:88:ASP:O	1:C:92:GLU:HG3	1.99	0.62
1:A:155:TRP:HE1	1:A:159:GLN:HG3	1.64	0.62
1:A:273:LEU:HD13	1:A:283:ILE:HG13	1.82	0.62
1:B:46:ILE:CD1	1:B:89:TRP:HB3	2.30	0.62
1:B:379:LEU:HD22	1:B:384:ASP:CB	2.22	0.62
1:A:58:ARG:HE	1:A:98:MET:HE2	1.64	0.62
1:C:225:TYR:OH	1:C:270:GLU:OE1	2.16	0.62
1:B:63:TRP:HZ3	1:B:101:LEU:HA	1.65	0.61
1:B:506:ASP:OD1	1:B:527:LYS:NZ	2.29	0.61
1:B:18:PRO:HG2	1:B:54:TYR:HA	1.82	0.61
1:B:373:GLN:HB2	1:B:415:THR:HB	1.83	0.61
1:C:7:THR:HB	1:C:10:GLN:HG3	1.82	0.61
1:B:408:LEU:HD11	1:B:432:ASP:HB2	1.82	0.61
1:B:232:VAL:HG23	1:B:234:VAL:HG23	1.81	0.61
1:B:351:ASP:OD2	1:B:406:GLY:N	2.33	0.60
1:B:381:LEU:HD23	1:B:381:LEU:C	2.22	0.60
1:A:207:HIS:CE1	1:A:211:LYS:HE3	2.36	0.60
1:A:155:TRP:NE1	1:A:159:GLN:HG3	2.17	0.60
1:C:12:TYR:HE1	1:C:142:MET:SD	2.25	0.60
1:A:506:ASP:HA	1:A:527:LYS:HG3	1.84	0.60
1:B:346:LEU:HD13	1:B:429:GLN:HG3	1.84	0.60
1:B:332:LYS:HA	1:B:335:TRP:CD1	2.38	0.59
1:B:332:LYS:HA	1:B:335:TRP:CG	2.37	0.59
1:A:58:ARG:NH1	1:A:270:GLU:OE1	2.35	0.59
1:C:273:LEU:HD13	1:C:283:ILE:HG13	1.83	0.59
1:A:44:GLU:O	1:A:48:THR:HG23	2.01	0.59
1:A:74:THR:HA	1:A:129:GLN:HE22	1.67	0.59
1:B:349:VAL:HG11	1:B:403:MET:SD	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:HIS:NE2	1:A:211:LYS:HE3	2.18	0.59
1:B:127:TRP:CE3	1:B:130:LEU:HD22	2.38	0.59
1:B:42:THR:HG22	1:B:44:GLU:N	2.17	0.58
1:B:125:ALA:O	1:B:129:GLN:HG2	2.02	0.58
1:C:194:LEU:HB3	1:C:202:LEU:HD22	1.84	0.58
1:C:408:LEU:HD13	1:C:453:ASN:HB3	1.86	0.58
1:C:100:ASN:HD21	1:C:102:HIS:HD2	1.52	0.57
1:A:115:ASN:ND2	1:A:118:GLU:OE1	2.24	0.57
1:B:174:TYR:CD2	1:B:213:LEU:HD22	2.39	0.56
1:B:241:GLU:CD	1:B:242:GLU:H	2.13	0.56
1:A:163:HIS:CG	1:A:205:ARG:HD2	2.40	0.56
1:A:282:VAL:HG13	1:A:481:PHE:HB3	1.86	0.56
1:A:349:VAL:HB	1:A:403:MET:HE1	1.87	0.56
1:A:46:ILE:HG22	1:A:93:GLU:HG3	1.86	0.56
1:A:184:ASN:OD1	1:A:187:ARG:NH1	2.37	0.56
1:C:461:GLU:HB2	1:C:512:THR:HB	1.88	0.56
1:A:372:LEU:HD23	1:A:416:ALA:HA	1.87	0.56
1:B:63:TRP:CZ3	1:B:101:LEU:HD23	2.41	0.56
1:B:50:ALA:HB2	1:B:95:LEU:HD11	1.88	0.56
1:C:142:MET:HG2	1:C:188:PRO:HB2	1.88	0.56
1:C:459:THR:HG22	1:C:460:MET:H	1.71	0.56
1:B:379:LEU:CD2	1:B:384:ASP:CG	2.47	0.55
1:B:115:ASN:ND2	1:B:118:GLU:OE1	2.32	0.55
1:B:252:PHE:HA	1:B:255:VAL:HG22	1.88	0.55
1:C:127:TRP:O	1:C:131:SER:OG	2.21	0.55
1:B:381:LEU:CD2	1:B:382:GLY:N	2.50	0.55
1:B:329:ASN:HA	1:B:332:LYS:HZ3	1.73	0.54
1:C:21:ASN:HB2	1:C:309:TRP:HA	1.88	0.54
1:A:150:ARG:HG2	1:A:195:GLU:HG2	1.90	0.54
1:B:198:THR:O	1:B:254:ARG:NH2	2.23	0.54
1:B:186:GLU:HB3	1:B:217:ASN:ND2	2.23	0.54
1:B:55:LYS:C	1:B:95:LEU:HD23	2.33	0.54
1:B:151:PHE:HD2	1:B:162:HIS:HD2	1.54	0.54
1:B:372:LEU:CD1	1:B:379:LEU:HB3	2.38	0.54
1:B:356:ARG:HG3	1:B:357:ASP:O	2.07	0.53
1:C:125:ALA:O	1:C:129:GLN:HG3	2.07	0.53
1:B:511:LEU:HD11	1:B:525:LEU:HD11	1.89	0.53
1:C:511:LEU:HD11	1:C:525:LEU:HD11	1.90	0.53
1:A:88:ASP:O	1:A:92:GLU:HG3	2.08	0.53
1:A:201:ASP:OD2	1:A:205:ARG:NH1	2.41	0.53
1:B:466:ASN:ND2	1:B:468:GLU:OE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ALA:HB3	1:B:479:LYS:HZ2	1.73	0.53
1:C:115:ASN:ND2	1:C:118:GLU:OE1	2.34	0.53
1:B:186:GLU:HB3	1:B:217:ASN:HD21	1.73	0.53
1:B:112:MET:SD	1:B:169:LEU:HD21	2.49	0.53
1:C:282:VAL:HG13	1:C:481:PHE:HB3	1.90	0.53
1:B:46:ILE:O	1:B:49:ILE:HG22	2.09	0.53
1:C:219:ILE:HG21	1:C:267:VAL:HG23	1.91	0.53
1:C:374:VAL:HG21	1:C:402:LEU:HD11	1.90	0.52
1:A:153:ARG:O	1:B:466:ASN:HB3	2.09	0.52
1:B:379:LEU:CD2	1:B:380:ALA:N	2.53	0.52
1:C:161:ASN:N	1:C:161:ASN:OD1	2.43	0.52
1:B:270:GLU:HG2	1:B:309:TRP:HB2	1.92	0.52
1:C:135:GLN:O	1:C:183:SER:HB2	2.09	0.52
1:A:245:GLN:HB3	1:A:294:PHE:CZ	2.45	0.52
1:B:342:ALA:HB2	1:B:426:PHE:HZ	1.74	0.52
1:B:379:LEU:HD23	1:B:380:ALA:CA	2.38	0.52
1:B:91:LEU:HD23	1:B:91:LEU:N	2.24	0.51
1:B:373:GLN:HE21	1:B:417:GLN:NE2	2.07	0.51
1:B:279:SER:O	1:B:282:VAL:HG22	2.09	0.51
1:C:66:GLN:HB3	1:C:76:ASN:HD22	1.76	0.51
1:B:380:ALA:O	1:B:384:ASP:HB2	2.10	0.51
1:C:245:GLN:HB3	1:C:294:PHE:CZ	2.45	0.51
1:A:167:GLU:O	1:A:171:THR:HG23	2.10	0.51
1:B:342:ALA:CB	1:B:426:PHE:CZ	2.90	0.51
1:A:207:HIS:CD2	1:A:211:LYS:HE3	2.45	0.51
1:B:149:PRO:HG2	1:B:194:LEU:HD12	1.92	0.51
1:B:173:PHE:CZ	1:B:189:LEU:HD22	2.46	0.51
1:B:473:GLN:CD	1:B:475:TRP:HE1	2.18	0.51
1:A:403:MET:HE3	1:A:428:LEU:HG	1.93	0.51
1:B:229:PRO:HB2	1:B:237:TYR:CD2	2.46	0.51
1:C:173:PHE:O	1:C:177:VAL:HG23	2.11	0.50
1:C:253:ASN:HD21	1:C:302:ARG:NH2	2.08	0.50
1:A:157:GLU:HB2	1:A:158:ILE:HG23	1.94	0.50
1:A:461:GLU:HG2	1:A:478:PHE:HA	1.93	0.50
1:A:511:LEU:HD11	1:A:525:LEU:HD11	1.92	0.50
1:A:173:PHE:O	1:A:177:VAL:HG23	2.11	0.50
1:B:80:PHE:O	1:B:83:VAL:HG22	2.11	0.50
1:B:264:ILE:HD12	1:B:265:PRO:HD2	1.93	0.50
1:B:372:LEU:O	1:B:378:SER:HA	2.12	0.50
1:C:404:THR:HB	1:C:407:GLU:HB2	1.94	0.50
1:B:285:GLN:NE2	1:B:324:ASP:OD2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:TYR:CE1	1:C:142:MET:SD	3.04	0.49
1:A:206:LEU:O	1:A:210:MET:HG3	2.12	0.49
1:A:84:GLU:HG3	1:A:134:PHE:CE1	2.46	0.49
1:B:350:ARG:HB3	1:B:353:GLU:HG2	1.95	0.49
1:C:58:ARG:NH1	1:C:144:GLU:OE1	2.46	0.49
1:A:506:ASP:OD1	1:A:527:LYS:HE3	2.12	0.49
1:B:173:PHE:CE1	1:B:177:VAL:HG21	2.48	0.49
1:C:106:TRP:HA	1:C:110:TYR:HB2	1.95	0.49
1:C:148:GLU:HA	1:C:196:THR:HG23	1.94	0.49
1:C:253:ASN:ND2	1:C:302:ARG:HH21	2.10	0.48
1:B:381:LEU:C	1:B:381:LEU:CD2	2.86	0.48
1:C:64:GLU:HA	1:C:67:MET:CE	2.43	0.48
1:C:332:LYS:HA	1:C:335:TRP:CD2	2.48	0.48
1:C:240:PHE:CZ	1:C:245:GLN:HG2	2.48	0.48
1:B:11:SER:O	1:B:15:ASP:HB2	2.14	0.48
1:B:106:TRP:CD1	1:B:106:TRP:H	2.32	0.48
1:B:505:ARG:HG3	1:B:507:ASP:HB2	1.95	0.48
1:B:93:GLU:HB2	1:B:95:LEU:HD12	1.96	0.48
1:C:100:ASN:HD21	1:C:102:HIS:CD2	2.31	0.48
1:B:471:GLY:H	1:B:504:VAL:HG12	1.79	0.48
1:B:379:LEU:CD2	1:B:379:LEU:C	2.86	0.48
1:C:7:THR:HG22	1:C:9:ILE:N	2.26	0.48
1:A:163:HIS:ND1	1:A:205:ARG:HD2	2.29	0.48
1:A:228:TRP:O	1:A:232:VAL:HG22	2.13	0.48
1:A:241:GLU:CG	1:A:242:GLU:H	2.27	0.48
1:B:64:GLU:OE1	1:B:107:LEU:HB3	2.13	0.48
1:B:461:GLU:HB2	1:B:512:THR:HB	1.95	0.48
1:B:172:ALA:O	1:B:176:ILE:HG12	2.14	0.47
1:A:12:TYR:CZ	1:A:188:PRO:HG2	2.49	0.47
1:A:16:MET:HB2	1:A:305:THR:HG21	1.95	0.47
1:B:215:ASP:HB3	1:B:218:LEU:HG	1.96	0.47
1:B:268:LEU:HD21	1:B:271:PHE:CB	2.36	0.47
1:C:77:GLU:CD	1:C:133:ARG:HH22	2.22	0.47
1:C:284:GLN:NE2	1:C:345:ASN:OD1	2.43	0.47
1:B:157:GLU:HB2	1:B:158:ILE:HG13	1.96	0.47
1:B:193:THR:HG21	1:B:197:ALA:O	2.15	0.47
1:B:9:ILE:HD13	1:B:217:ASN:HA	1.97	0.47
1:C:9:ILE:HG23	1:C:265:PRO:HG3	1.95	0.47
1:C:46:ILE:HG22	1:C:93:GLU:HG3	1.96	0.47
1:C:100:ASN:ND2	1:C:102:HIS:HD2	2.11	0.47
1:A:125:ALA:O	1:A:129:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:HIS:NE2	1:A:211:LYS:CE	2.78	0.47
1:A:466:ASN:HB3	1:B:153:ARG:O	2.15	0.47
1:B:23:GLY:HA3	1:B:309:TRP:HZ3	1.74	0.47
1:A:155:TRP:CZ2	1:A:159:GLN:HB2	2.50	0.47
1:B:163:HIS:ND1	1:B:205:ARG:HD2	2.30	0.47
1:B:173:PHE:HE1	1:B:177:VAL:HG21	1.79	0.47
1:A:232:VAL:HG23	1:A:234:VAL:HG23	1.96	0.47
1:B:209:THR:O	1:B:213:LEU:HG	2.14	0.46
1:A:241:GLU:HG3	1:A:242:GLU:H	1.80	0.46
1:B:22:LEU:HD21	1:B:41:VAL:HG11	1.96	0.46
1:B:408:LEU:CD1	1:B:432:ASP:HB2	2.45	0.46
1:A:48:THR:HG21	1:A:320:TYR:HB3	1.98	0.46
1:B:174:TYR:CE2	1:B:213:LEU:HB3	2.50	0.46
1:A:21:ASN:HB2	1:A:309:TRP:HA	1.98	0.46
1:B:248:ILE:HG12	1:B:295:LEU:HD23	1.98	0.46
1:A:490:ASP:OD1	1:A:490:ASP:N	2.41	0.46
1:B:165:PHE:O	1:B:169:LEU:HD23	2.16	0.46
1:B:295:LEU:HD13	1:B:299:LEU:HD11	1.97	0.46
1:B:91:LEU:HD22	1:B:95:LEU:O	2.15	0.46
1:C:206:LEU:HG	1:C:210:MET:HE3	1.98	0.46
1:A:135:GLN:O	1:A:183:SER:HB2	2.16	0.46
1:C:27:ASP:O	1:C:103:HIS:HD2	1.99	0.46
1:B:33:GLU:CD	1:B:82:ARG:HE	2.23	0.45
1:B:135:GLN:O	1:B:183:SER:HB2	2.16	0.45
1:B:55:LYS:O	1:B:96:TYR:HD1	1.99	0.45
1:B:151:PHE:HD2	1:B:162:HIS:CD2	2.34	0.45
1:B:350:ARG:HA	1:B:431:VAL:O	2.16	0.45
1:B:102:HIS:HD2	1:B:103:HIS:CD2	2.34	0.45
1:B:379:LEU:CG	1:B:384:ASP:OD2	2.59	0.45
1:C:171:THR:HA	1:C:213:LEU:HD21	1.99	0.45
1:A:98:MET:HA	1:A:142:MET:HG2	1.97	0.45
1:A:27:ASP:HB2	1:A:102:HIS:CD2	2.51	0.45
1:B:184:ASN:HA	1:B:187:ARG:HB2	1.97	0.45
1:B:151:PHE:CD2	1:B:162:HIS:HD2	2.33	0.45
1:B:158:ILE:HG22	1:B:159:GLN:N	2.31	0.45
1:B:102:HIS:CD2	1:B:103:HIS:CD2	3.05	0.45
1:A:27:ASP:HB2	1:A:102:HIS:HD2	1.82	0.44
1:B:310:ASP:OD2	1:B:314:HIS:HB2	2.17	0.44
1:B:289:LEU:HD11	1:B:326:GLU:OE2	2.17	0.44
1:B:381:LEU:HD23	1:B:382:GLY:CA	2.42	0.44
1:A:27:ASP:O	1:A:103:HIS:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TYR:CZ	1:B:188:PRO:HG2	2.52	0.44
1:A:106:TRP:HA	1:A:110:TYR:HB2	1.98	0.44
1:A:161:ASN:OD1	1:A:161:ASN:N	2.49	0.44
1:B:145:SER:OG	1:B:146:VAL:N	2.51	0.44
1:C:98:MET:SD	1:C:144:GLU:HB2	2.57	0.44
1:A:464:TYR:CE1	1:A:505:ARG:HG2	2.53	0.44
1:B:271:PHE:HE1	1:B:306:HIS:ND1	2.16	0.44
1:B:175:HIS:O	1:B:179:GLU:HB2	2.18	0.44
1:C:364:LEU:HB3	1:C:367:ASN:O	2.18	0.44
1:B:127:TRP:CZ3	1:B:143:PHE:HB3	2.53	0.44
1:B:286:GLY:HA3	1:B:345:ASN:HB2	1.99	0.44
1:B:411:ASN:OD1	1:B:430:ASN:HB2	2.18	0.44
1:C:285:GLN:NE2	1:C:324:ASP:OD2	2.46	0.44
1:A:151:PHE:HB2	1:A:162:HIS:CD2	2.53	0.44
1:C:58:ARG:HD2	1:C:98:MET:HE3	2.00	0.44
1:C:157:GLU:HA	1:C:158:ILE:HA	1.64	0.43
1:A:157:GLU:HB2	1:A:158:ILE:CG2	2.48	0.43
1:B:48:THR:HG21	1:B:320:TYR:HB3	2.00	0.43
1:B:362:LEU:HD11	1:B:392:LEU:HB3	1.99	0.43
1:B:373:GLN:HE21	1:B:417:GLN:HE21	1.65	0.43
1:C:473:GLN:OE1	1:C:475:TRP:NE1	2.31	0.43
1:B:164:ALA:O	1:B:168:GLU:HG3	2.18	0.43
1:B:210:MET:HG2	1:B:218:LEU:HD13	2.00	0.43
1:B:501:PHE:HA	1:B:504:VAL:HG22	2.01	0.43
1:C:64:GLU:HA	1:C:67:MET:HE3	1.99	0.43
1:B:13:VAL:HG11	1:B:265:PRO:HB2	2.01	0.43
1:C:533:GLN:NE2	1:C:535:ARG:HD2	2.33	0.43
1:A:106:TRP:CD1	1:A:106:TRP:H	2.37	0.43
1:A:505:ARG:O	1:A:527:LYS:HG2	2.18	0.43
1:B:196:THR:HB	1:B:223:HIS:H	1.83	0.43
1:B:245:GLN:HB3	1:B:294:PHE:CZ	2.53	0.43
1:B:32:ASP:OD2	1:B:34:THR:HG22	2.19	0.43
1:B:334:SER:HA	1:B:337:GLY:O	2.18	0.43
1:C:241:GLU:OE2	1:C:243:GLU:HB2	2.19	0.43
1:C:96:TYR:CZ	1:C:140:LYS:HE3	2.54	0.43
1:B:369:LEU:HD12	1:B:417:GLN:O	2.19	0.42
1:B:386:GLU:OE2	1:B:395:LYS:HE2	2.19	0.42
1:C:163:HIS:CG	1:C:205:ARG:HD2	2.54	0.42
1:B:13:VAL:HG21	1:B:265:PRO:HG2	2.01	0.42
1:B:127:TRP:CZ3	1:B:130:LEU:HD22	2.54	0.42
1:B:138:SER:OG	1:B:140:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASN:HB2	1:C:308:LEU:O	2.19	0.42
1:A:505:ARG:HG3	1:A:507:ASP:HB2	2.00	0.42
1:B:105:SER:HB2	1:B:147:ASN:O	2.20	0.42
1:B:504:VAL:HG23	1:B:527:LYS:HD3	2.01	0.42
1:A:202:LEU:HD22	1:A:202:LEU:H	1.85	0.42
1:B:127:TRP:CZ3	1:B:173:PHE:CE1	3.08	0.42
1:B:251:THR:O	1:B:255:VAL:HG13	2.19	0.42
1:C:104:ASP:HA	1:C:107:LEU:HB2	2.00	0.42
1:C:154:ASP:N	1:C:159:GLN:OE1	2.47	0.42
1:C:84:GLU:HG3	1:C:134:PHE:CE1	2.55	0.42
1:C:459:THR:HG22	1:C:460:MET:N	2.34	0.42
1:C:466:ASN:ND2	1:C:468:GLU:OE1	2.48	0.42
1:C:201:ASP:OD2	1:C:205:ARG:NH1	2.53	0.42
1:A:380:ALA:O	1:A:384:ASP:HB2	2.20	0.42
1:B:123:TYR:CE1	1:B:169:LEU:HD12	2.55	0.42
1:A:164:ALA:O	1:A:168:GLU:HG3	2.20	0.42
1:A:372:LEU:HD12	1:A:385:TYR:CG	2.55	0.42
1:C:43:ARG:NH2	1:C:93:GLU:OE2	2.52	0.42
1:C:372:LEU:HD12	1:C:385:TYR:CD1	2.55	0.42
1:C:504:VAL:HG12	1:C:527:LYS:HD3	2.01	0.42
1:A:158:ILE:HB	1:A:162:HIS:ND1	2.35	0.41
1:A:194:LEU:HB3	1:A:202:LEU:HD12	2.02	0.41
1:A:315:LEU:HB2	1:A:322:TRP:CE3	2.55	0.41
1:B:17:GLN:HA	1:B:18:PRO:HA	1.84	0.41
1:B:342:ALA:HB3	1:B:426:PHE:CZ	2.55	0.41
1:C:7:THR:CG2	1:C:9:ILE:HG22	2.50	0.41
1:C:198:THR:OG1	1:C:251:THR:HG23	2.20	0.41
1:A:174:TYR:OH	1:A:215:ASP:HB2	2.19	0.41
1:B:239:ARG:HE	1:B:239:ARG:HB3	1.25	0.41
1:C:177:VAL:HG11	1:C:189:LEU:HD21	2.01	0.41
1:C:210:MET:SD	1:C:264:ILE:HD13	2.60	0.41
1:C:229:PRO:HA	1:C:234:VAL:HG12	2.02	0.41
1:A:58:ARG:HH21	1:A:144:GLU:CD	2.27	0.41
1:B:178:ARG:HA	1:B:178:ARG:HD3	1.74	0.41
1:B:202:LEU:HA	1:B:205:ARG:HG3	2.02	0.41
1:B:346:LEU:CD1	1:B:429:GLN:HG3	2.50	0.41
1:B:367:ASN:CG	1:B:420:SER:HB3	2.45	0.41
1:A:115:ASN:O	1:A:119:VAL:HG13	2.20	0.41
1:A:350:ARG:NH1	1:A:519:GLU:OE2	2.45	0.41
1:B:178:ARG:HD3	1:B:178:ARG:HH11	1.75	0.41
1:C:386:GLU:OE1	1:C:395:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TYR:HE2	1:A:218:LEU:HD21	1.85	0.41
1:A:174:TYR:CE1	1:A:178:ARG:HG3	2.56	0.41
1:B:316:ASN:CG	1:B:319:THR:HG23	2.46	0.41
1:C:174:TYR:CD1	1:C:213:LEU:HD23	2.56	0.41
1:A:158:ILE:HG21	1:A:194:LEU:HD21	2.03	0.41
1:A:403:MET:HE2	1:A:430:ASN:HB2	2.01	0.41
1:B:373:GLN:HG3	1:B:417:GLN:NE2	2.35	0.41
1:C:102:HIS:HB3	1:C:103:HIS:H	1.74	0.41
1:B:360:ILE:CD1	1:B:426:PHE:CD2	2.99	0.41
1:A:60:PRO:HA	1:A:100:ASN:OD1	2.21	0.41
1:A:372:LEU:HD12	1:A:385:TYR:CD1	2.56	0.41
1:B:360:ILE:HD13	1:B:360:ILE:HG21	1.88	0.41
1:C:7:THR:HG21	1:C:9:ILE:HG22	2.02	0.41
1:C:461:GLU:O	1:C:511:LEU:HA	2.21	0.41
1:B:184:ASN:OD1	1:B:187:ARG:NH2	2.54	0.41
1:B:282:VAL:HG23	1:B:283:ILE:HD12	2.02	0.41
1:B:315:LEU:HB2	1:B:322:TRP:CE3	2.56	0.41
1:C:197:ALA:HB3	1:C:202:LEU:HD13	2.03	0.41
1:B:100:ASN:HA	1:B:144:GLU:O	2.21	0.40
1:A:479:LYS:HD3	1:A:479:LYS:HA	1.61	0.40
1:A:158:ILE:HD12	1:A:158:ILE:C	2.46	0.40
1:C:60:PRO:HA	1:C:100:ASN:OD1	2.21	0.40
1:A:174:TYR:C	1:A:174:TYR:CD1	3.00	0.40
1:B:13:VAL:HG22	1:B:16:MET:HE3	2.03	0.40
1:B:240:PHE:CZ	1:B:245:GLN:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	529/585 (90%)	507 (96%)	21 (4%)	1 (0%)	43 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	528/585 (90%)	500 (95%)	28 (5%)	0	100	100
1	C	530/585 (91%)	505 (95%)	24 (4%)	1 (0%)	43	72
All	All	1587/1755 (90%)	1512 (95%)	73 (5%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	70	ALA
1	A	160	GLU

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	462/503 (92%)	461 (100%)	1 (0%)	87	96
1	B	461/503 (92%)	461 (100%)	0	100	100
1	C	463/503 (92%)	463 (100%)	0	100	100
All	All	1386/1509 (92%)	1385 (100%)	1 (0%)	88	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	207	HIS
1	A	245	GLN
1	A	262	ASN
1	A	306	HIS
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	427	GLN
1	A	438	ASN
1	B	10	GLN
1	B	85	GLN
1	B	135	GLN
1	B	162	HIS
1	B	217	ASN
1	B	345	ASN
1	B	363	HIS
1	B	373	GLN
1	B	510	HIS
1	B	533	GLN
1	C	66	GLN
1	C	76	ASN
1	C	102	HIS
1	C	129	GLN
1	C	135	GLN
1	C	200	GLN
1	C	204	ASN
1	C	253	ASN
1	C	313	GLN
1	C	361	GLN
1	C	411	ASN
1	C	417	GLN
1	C	438	ASN
1	C	510	HIS
1	C	533	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	308:LEU	C	309:TRP	N	1.13

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	531/585 (90%)	0.76	23 (4%) 40 31	26, 55, 82, 119	0
1	B	530/585 (90%)	2.80	416 (78%) 0 0	30, 90, 108, 126	0
1	C	532/585 (90%)	0.58	16 (3%) 52 43	14, 28, 49, 83	0
All	All	1593/1755 (90%)	1.38	455 (28%) 1 1	14, 56, 101, 126	0

All (455) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	ALA	6.6
1	B	389	GLY	5.9
1	B	372	LEU	5.9
1	B	521	VAL	5.3
1	B	306	HIS	5.2
1	B	426	PHE	5.1
1	B	366	GLY	5.1
1	B	416	ALA	5.1
1	B	385	TYR	5.0
1	B	274	LEU	4.9
1	B	130	LEU	4.9
1	B	360	ILE	4.8
1	B	424	TRP	4.8
1	B	111	ASN	4.8
1	B	102	HIS	4.8
1	C	155	TRP	4.7
1	B	107	LEU	4.7
1	B	346	LEU	4.7
1	B	57	ILE	4.7
1	B	189	LEU	4.7
1	B	428	LEU	4.7
1	B	413	VAL	4.7
1	B	364	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	252	PHE	4.6
1	B	309	TRP	4.6
1	B	176	ILE	4.5
1	B	271	PHE	4.5
1	B	14	ALA	4.4
1	B	236	GLY	4.4
1	B	259	PHE	4.4
1	B	41	VAL	4.4
1	B	210	MET	4.4
1	B	388	ALA	4.4
1	B	340	ALA	4.3
1	B	242	GLU	4.3
1	B	162	HIS	4.3
1	B	90	ALA	4.3
1	B	304	VAL	4.3
1	B	345	ASN	4.3
1	B	411	ASN	4.3
1	B	313	GLN	4.3
1	B	520	MET	4.3
1	B	194	LEU	4.3
1	B	414	ILE	4.3
1	B	142	MET	4.3
1	A	465	ALA	4.3
1	B	251	THR	4.2
1	B	479	LYS	4.2
1	B	348	HIS	4.2
1	A	156	GLY	4.2
1	B	342	ALA	4.1
1	B	260	THR	4.1
1	B	155	TRP	4.1
1	B	212	ASP	4.1
1	B	427	GLN	4.1
1	B	381	LEU	4.1
1	B	367	ASN	4.1
1	B	138	SER	4.1
1	B	339	SER	4.1
1	B	365	HIS	4.1
1	B	237	TYR	4.1
1	B	390	ASP	4.0
1	B	282	VAL	4.0
1	B	97	VAL	4.0
1	B	341	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	198	THR	4.0
1	B	524	THR	4.0
1	B	347	ILE	3.9
1	B	127	TRP	3.9
1	B	206	LEU	3.9
1	B	217	ASN	3.9
1	B	425	HIS	3.9
1	B	275	GLY	3.9
1	B	220	ALA	3.9
1	B	136	GLY	3.8
1	B	182	GLY	3.8
1	B	160	GLU	3.8
1	B	21	ASN	3.8
1	C	69	ASN	3.8
1	B	276	PHE	3.8
1	B	13	VAL	3.8
1	A	111	ASN	3.8
1	B	286	GLY	3.8
1	B	125	ALA	3.7
1	B	147	ASN	3.7
1	B	188	PRO	3.7
1	B	379	LEU	3.7
1	B	173	PHE	3.7
1	B	421	GLY	3.7
1	B	404	THR	3.7
1	B	15	ASP	3.7
1	B	230	PHE	3.7
1	B	338	ARG	3.7
1	B	29	VAL	3.7
1	B	344	SER	3.7
1	B	139	HIS	3.7
1	B	169	LEU	3.7
1	B	336	GLU	3.7
1	B	403	MET	3.6
1	A	155	TRP	3.6
1	B	386	GLU	3.6
1	B	307	MET	3.6
1	B	63	TRP	3.6
1	B	391	VAL	3.6
1	B	370	THR	3.6
1	B	459	THR	3.6
1	B	16	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	332	LYS	3.6
1	B	272	GLY	3.6
1	B	167	GLU	3.6
1	C	157	GLU	3.6
1	B	363	HIS	3.6
1	B	109	ILE	3.6
1	B	177	VAL	3.6
1	B	186	GLU	3.6
1	B	22	LEU	3.6
1	B	141	LEU	3.6
1	B	258	THR	3.6
1	B	331	LEU	3.6
1	B	17	GLN	3.5
1	B	292	PHE	3.5
1	B	296	ILE	3.5
1	B	457	VAL	3.5
1	B	54	TYR	3.5
1	B	244	THR	3.5
1	B	284	GLN	3.5
1	B	333	ALA	3.5
1	B	158	ILE	3.5
1	B	56	SER	3.5
1	B	7	THR	3.5
1	B	219	ILE	3.5
1	B	83	VAL	3.5
1	B	514	HIS	3.5
1	B	264	ILE	3.5
1	B	374	VAL	3.5
1	B	273	LEU	3.5
1	B	145	SER	3.5
1	B	170	ASN	3.5
1	B	227	PHE	3.4
1	B	146	VAL	3.4
1	B	270	GLU	3.4
1	B	410	THR	3.4
1	B	98	MET	3.4
1	B	222	VAL	3.4
1	B	50	ALA	3.4
1	B	225	TYR	3.4
1	B	288	LYS	3.4
1	B	518	GLY	3.4
1	B	20	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	48	THR	3.4
1	B	101	LEU	3.4
1	A	160	GLU	3.4
1	B	354	PRO	3.4
1	B	434	PRO	3.4
1	B	239	ARG	3.3
1	B	149	PRO	3.3
1	B	470	ALA	3.3
1	B	166	LEU	3.3
1	B	369	LEU	3.3
1	B	475	TRP	3.3
1	B	266	VAL	3.3
1	B	100	ASN	3.3
1	B	99	LEU	3.3
1	B	387	LEU	3.3
1	B	513	PHE	3.3
1	B	382	GLY	3.3
1	B	422	ALA	3.3
1	C	142	MET	3.3
1	B	49	ILE	3.3
1	B	256	HIS	3.3
1	B	362	LEU	3.3
1	B	327	PHE	3.3
1	B	535	ARG	3.3
1	B	278	THR	3.3
1	B	435	THR	3.3
1	B	140	LYS	3.2
1	B	255	VAL	3.2
1	B	323	TYR	3.2
1	B	357	ASP	3.2
1	B	335	TRP	3.2
1	B	343	GLU	3.2
1	B	407	GLU	3.2
1	B	11	SER	3.2
1	B	12	TYR	3.2
1	B	191	LEU	3.2
1	B	103	HIS	3.2
1	B	245	GLN	3.2
1	B	417	GLN	3.2
1	B	34	THR	3.2
1	A	526	SER	3.2
1	B	308	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	121	ALA	3.2
1	B	143	PHE	3.2
1	B	418	PHE	3.2
1	B	337	GLY	3.2
1	B	305	THR	3.2
1	A	158	ILE	3.2
1	B	261	ALA	3.1
1	B	137	HIS	3.1
1	B	175	HIS	3.1
1	B	42	THR	3.1
1	B	355	ILE	3.1
1	B	405	PRO	3.1
1	B	295	LEU	3.1
1	B	444	SER	3.1
1	B	134	PHE	3.1
1	B	39	PRO	3.1
1	B	265	PRO	3.1
1	B	213	LEU	3.1
1	B	80	PHE	3.1
1	B	123	TYR	3.1
1	B	234	VAL	3.1
1	B	199	SER	3.1
1	B	384	ASP	3.1
1	B	420	SER	3.1
1	B	161	ASN	3.1
1	B	233	ASN	3.1
1	B	412	ALA	3.0
1	B	226	GLY	3.0
1	B	62	THR	3.0
1	B	197	ALA	3.0
1	B	106	TRP	3.0
1	B	526	SER	3.0
1	B	178	ARG	3.0
1	B	249	ILE	3.0
1	B	371	GLY	3.0
1	B	290	LYS	3.0
1	B	126	LEU	3.0
1	B	218	LEU	3.0
1	A	440	GLU	3.0
1	B	18	PRO	3.0
1	B	519	GLU	3.0
1	B	25	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	452	PHE	3.0
1	B	65	ASN	3.0
1	B	120	MET	3.0
1	B	458	ALA	3.0
1	B	478	PHE	3.0
1	B	89	TRP	2.9
1	B	516	TRP	2.9
1	B	27	ASP	2.9
1	B	330	MET	2.9
1	B	61	VAL	2.9
1	B	415	THR	2.9
1	A	536	ARG	2.9
1	B	529	GLY	2.9
1	B	368	GLU	2.9
1	B	311	ASN	2.9
1	B	474	ASN	2.9
1	B	280	THR	2.9
1	B	150	ARG	2.9
1	B	254	ARG	2.9
1	B	59	ILE	2.9
1	B	268	LEU	2.9
1	C	160	GLU	2.9
1	B	267	VAL	2.9
1	B	10	GLN	2.9
1	B	334	SER	2.9
1	B	297	HIS	2.9
1	B	209	THR	2.9
1	B	283	ILE	2.9
1	B	392	LEU	2.9
1	B	402	LEU	2.9
1	C	156	GLY	2.8
1	B	325	GLN	2.8
1	B	232	VAL	2.8
1	B	187	ARG	2.8
1	B	350	ARG	2.8
1	B	517	SER	2.8
1	B	66	GLN	2.8
1	B	51	ASP	2.8
1	B	207	HIS	2.8
1	C	76	ASN	2.8
1	B	393	THR	2.8
1	B	156	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	373	GLN	2.8
1	B	58	ARG	2.8
1	A	512	THR	2.8
1	B	60	PRO	2.8
1	B	104	ASP	2.8
1	B	152	THR	2.8
1	B	269	GLY	2.8
1	B	302	ARG	2.7
1	B	440	GLU	2.7
1	A	228	TRP	2.7
1	B	228	TRP	2.7
1	B	436	LEU	2.7
1	B	298	HIS	2.7
1	B	94	ASP	2.7
1	B	81	SER	2.7
1	B	321	SER	2.7
1	B	129	GLN	2.7
1	B	9	ILE	2.7
1	B	108	TRP	2.7
1	B	451	HIS	2.7
1	B	460	MET	2.7
1	A	508	ASP	2.7
1	C	490	ASP	2.7
1	B	536	ARG	2.7
1	B	113	GLU	2.7
1	B	241	GLU	2.7
1	B	46	ILE	2.7
1	B	240	PHE	2.7
1	A	112	MET	2.7
1	B	314	HIS	2.7
1	B	95	LEU	2.7
1	B	35	ALA	2.7
1	B	165	PHE	2.7
1	B	291	PHE	2.7
1	B	450	ALA	2.7
1	B	53	GLY	2.7
1	B	353	GLU	2.7
1	B	431	VAL	2.7
1	B	378	SER	2.7
1	B	185	THR	2.6
1	B	47	LYS	2.6
1	B	105	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	465	ALA	2.6
1	A	464	TYR	2.6
1	B	96	TYR	2.6
1	B	45	LEU	2.6
1	B	522	GLU	2.6
1	B	26	PHE	2.6
1	B	299	LEU	2.6
1	B	400	THR	2.6
1	B	303	ASP	2.6
1	A	162	HIS	2.6
1	A	524	THR	2.6
1	B	75	ILE	2.6
1	B	86	VAL	2.6
1	B	168	GLU	2.6
1	B	419	ASN	2.6
1	B	423	ASP	2.6
1	B	163	HIS	2.5
1	B	30	GLY	2.5
1	B	71	PRO	2.5
1	B	263	GLY	2.5
1	B	190	VAL	2.5
1	B	489	TYR	2.5
1	B	171	THR	2.5
1	B	179	GLU	2.5
1	B	293	GLU	2.5
1	B	43	ARG	2.5
1	B	69	ASN	2.5
1	B	8	ASP	2.5
1	B	277	ASP	2.5
1	A	120	MET	2.5
1	C	241	GLU	2.5
1	B	358	GLN	2.5
1	B	24	ASN	2.5
1	B	223	HIS	2.5
1	B	329	ASN	2.5
1	A	509	ILE	2.5
1	B	84	GLU	2.5
1	B	224	TYR	2.5
1	B	447	ALA	2.5
1	B	151	PHE	2.4
1	B	287	GLU	2.4
1	B	110	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	361	GLN	2.4
1	B	193	THR	2.4
1	B	114	HIS	2.4
1	B	91	LEU	2.4
1	B	289	LEU	2.4
1	B	44	GLU	2.4
1	B	135	GLN	2.4
1	B	221	THR	2.4
1	B	112	MET	2.4
1	B	211	LYS	2.4
1	B	485	PHE	2.4
1	B	36	TRP	2.4
1	B	208	GLN	2.4
1	B	253	ASN	2.4
1	B	248	ILE	2.4
1	B	481	PHE	2.3
1	B	322	TRP	2.3
1	B	124	THR	2.3
1	B	523	TYR	2.3
1	B	432	ASP	2.3
1	B	396	ALA	2.3
1	B	511	LEU	2.3
1	A	510	HIS	2.3
1	B	19	GLY	2.3
1	B	23	GLY	2.3
1	B	157	GLU	2.3
1	B	359	ASP	2.3
1	B	473	GLN	2.3
1	C	309	TRP	2.3
1	B	238	THR	2.3
1	B	454	GLY	2.3
1	B	64	GLU	2.3
1	B	67	MET	2.2
1	B	203	LEU	2.2
1	B	159	GLN	2.2
1	B	246	GLN	2.2
1	B	351	ASP	2.2
1	B	180	SER	2.2
1	B	183	SER	2.2
1	B	181	GLY	2.2
1	B	195	GLU	2.2
1	B	383	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	300	ASN	2.2
1	B	281	ASP	2.2
1	B	375	ASP	2.2
1	B	216	PRO	2.2
1	B	476	THR	2.2
1	B	488	VAL	2.2
1	B	279	SER	2.2
1	B	164	ALA	2.2
1	B	262	ASN	2.2
1	B	32	ASP	2.2
1	B	192	PRO	2.2
1	B	487	PRO	2.2
1	B	409	GLY	2.2
1	B	477	SER	2.2
1	B	486	SER	2.2
1	B	33	GLU	2.2
1	B	52	GLU	2.2
1	B	508	ASP	2.2
1	B	406	GLY	2.2
1	B	401	ALA	2.2
1	A	114	HIS	2.1
1	B	204	ASN	2.1
1	B	445	ASN	2.1
1	B	196	THR	2.1
1	B	471	GLY	2.1
1	B	525	LEU	2.1
1	B	464	TYR	2.1
1	A	533	GLN	2.1
1	B	184	ASN	2.1
1	B	376	GLY	2.1
1	C	121	ALA	2.1
1	B	243	GLU	2.1
1	B	430	ASN	2.1
1	B	449	PRO	2.1
1	B	312	GLY	2.1
1	B	319	THR	2.1
1	B	82	ARG	2.1
1	B	128	GLU	2.1
1	A	517	SER	2.1
1	C	6	GLN	2.1
1	B	467	GLY	2.1
1	B	442	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	528	ASN	2.0
1	B	408	LEU	2.0
1	B	294	PHE	2.0
1	C	78	ASP	2.0
1	C	5	LYS	2.0
1	B	153	ARG	2.0
1	B	214	ASN	2.0
1	C	111	ASN	2.0
1	B	509	ILE	2.0
1	C	185	THR	2.0
1	B	116	TYR	2.0
1	B	174	TYR	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.