



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:17 AM EDT

PDB ID : 5XRC
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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

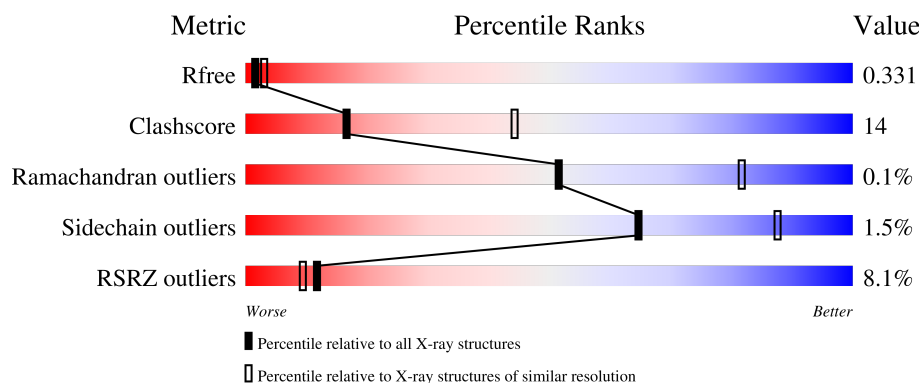
1 Overall quality at a glance

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>9%</div> </div> </div>
1	B	585	<div> <div>20%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>9%</div> </div> </div>
1	C	585	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>9%</div> </div> </div>

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

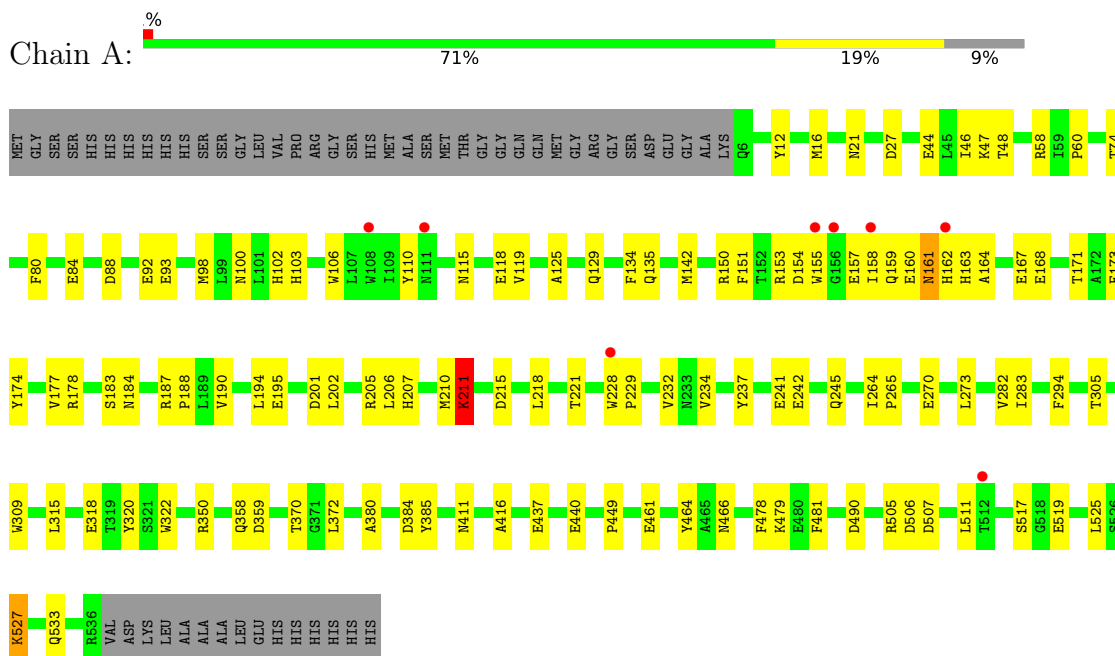
- Molecule 2 is water.

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

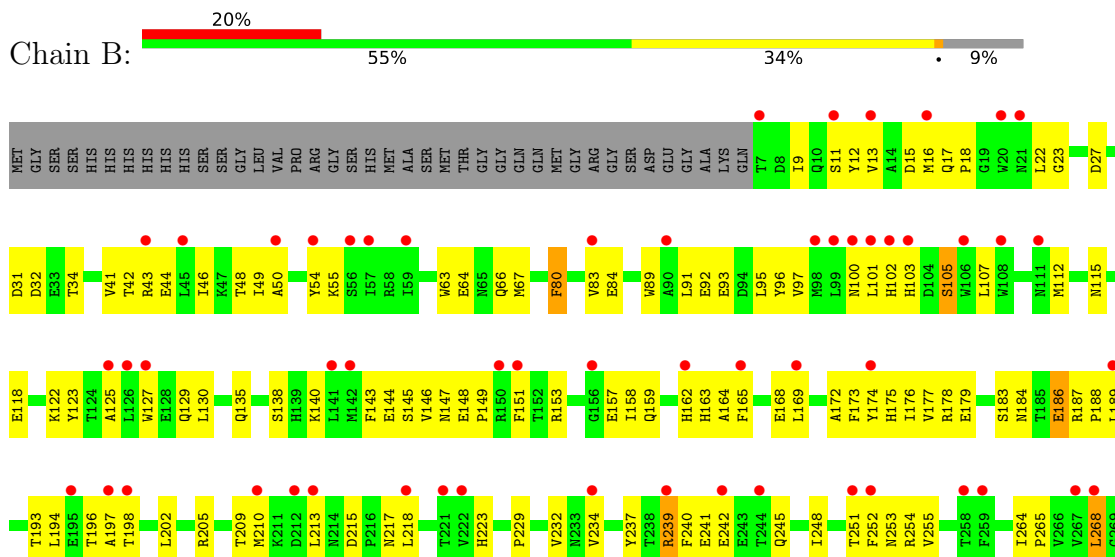
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cellulase



• 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 0.277 , 0.331	Depositor DCC
R_{free} test set	2408 reflections (4.78%)	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)	0.34 , 58.9	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	0.30	0/4430	0.53	2/6032 (0.0%)
1	B	0.37	1/4421 (0.0%)	0.64	6/6020 (0.1%)
1	C	0.30	1/4439 (0.0%)	0.53	2/6043 (0.0%)
All	All	0.33	2/13290 (0.0%)	0.57	10/18095 (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	-9.01	1.13	1.34
1	B	186	GLU	CB-CG	6.95	1.65	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	309	TRP	O-C-N	10.00	138.70	122.70
1	B	239	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	C	309	TRP	CA-C-N	-7.82	99.99	117.20
1	A	211	LYS	CA-CB-CG	7.51	129.93	113.40
1	B	239	ARG	CG-CD-NE	-7.41	96.25	111.80
1	B	372	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	318	GLU	CA-CB-CG	5.87	126.31	113.40
1	B	239	ARG	CA-CB-CG	5.77	126.09	113.40
1	B	346	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	B	295	LEU	CA-CB-CG	5.17	127.20	115.30

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	83	0
1	B	4303	0	3968	189	0
1	C	4321	0	3988	83	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	353	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 14.

All (353) 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	1.30
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:A:58:ARG:HE	1:A:98:MET:HE2	1.61	0.65
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:225:TYR:OH	1:C:270:GLU:OE1	2.16	0.62
1:B:379:LEU:HD23	1:B:379:LEU:C	2.19	0.62
1:B:63:TRP:HZ3	1:B:101:LEU:HA	1.65	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: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:B:506:ASP:OD1	1:B:527:LYS:NZ	2.29	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
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: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:46:ILE:HG22	1:A:93:GLU:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:381:LEU:HD23	1:B:381:LEU:C	2.22	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: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: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
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:241:GLU:CD	1:B:242:GLU:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:55:LYS:C	1:B:95:LEU:HD23	2.33	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:B:473:GLN:CD	1:B:475:TRP:HE1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:13:VAL:HA	1:B:16:MET:HE2	1.98	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
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:B:381:LEU:C	1:B:381:LEU:CD2	2.86	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:CD2	1:B:379:LEU:C	2.86	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: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: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:77:GLU:CD	1:C:133:ARG:HH22	2.22	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:B:462:ALA:HB3	1:B:479:LYS:HZ2	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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:C:60:PRO:HA	1:C:100:ASN:OD1	2.21	0.40
1:B:67:MET:HE1	1:B:122:LYS:HB3	2.04	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 [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	529/585 (90%)	507 (96%)	21 (4%)	1 (0%)	47	78
1	B	528/585 (90%)	500 (95%)	28 (5%)	0	100	100
1	C	530/585 (91%)	505 (95%)	24 (4%)	1 (0%)	47	78
All	All	1587/1755 (90%)	1512 (95%)	73 (5%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

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

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	462/503 (92%)	453 (98%)	9 (2%)	57	84
1	B	461/503 (92%)	452 (98%)	9 (2%)	55	82
1	C	463/503 (92%)	460 (99%)	3 (1%)	86	96
All	All	1386/1509 (92%)	1365 (98%)	21 (2%)	65	87

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	80	PHE
1	A	161	ASN
1	A	211	LYS
1	A	358	GLN
1	A	359	ASP
1	A	411	ASN
1	A	517	SER
1	A	527	LYS
1	B	43	ARG
1	B	80	PHE
1	B	84	GLU
1	B	105	SER
1	B	268	LEU
1	B	332	LYS
1	B	346	LEU
1	B	359	ASP
1	B	517	SER
1	C	76	ASN
1	C	80	PHE
1	C	361	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	207	HIS
1	A	245	GLN
1	A	262	ASN
1	A	438	ASN
1	A	533	GLN
1	B	217	ASN
1	B	345	ASN
1	B	365	HIS
1	B	417	GLN
1	C	76	ASN
1	C	102	HIS
1	C	253	ASN
1	C	411	ASN
1	C	425	HIS
1	C	438	ASN

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 monosaccharides 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%)	0.44	8 (1%) 73 73	26, 55, 82, 119	0
1	B	530/585 (90%)	1.34	117 (22%) 0 0	30, 90, 108, 126	0
1	C	532/585 (90%)	0.27	4 (0%) 86 86	14, 28, 49, 83	0
All	All	1593/1755 (90%)	0.68	129 (8%) 12 9	14, 56, 101, 126	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	414	ILE	4.4
1	B	426	PHE	3.8
1	B	99	LEU	3.7
1	B	57	ILE	3.6
1	B	90	ALA	3.6
1	B	212	ASP	3.6
1	B	141	LEU	3.6
1	B	335	TRP	3.4
1	B	389	GLY	3.4
1	A	158	ILE	3.3
1	A	111	ASN	3.3
1	B	424	TRP	3.3
1	B	388	ALA	3.3
1	B	296	ILE	3.2
1	B	101	LEU	3.2
1	B	259	PHE	3.1
1	B	127	TRP	3.1
1	B	242	GLU	3.1
1	B	252	PHE	3.1
1	B	276	PHE	3.0
1	B	7	THR	3.0
1	B	111	ASN	3.0
1	B	102	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	348	HIS	3.0
1	B	13	VAL	2.9
1	B	304	VAL	2.9
1	B	309	TRP	2.9
1	B	521	VAL	2.9
1	B	282	VAL	2.9
1	B	125	ALA	2.8
1	B	427	GLN	2.8
1	B	16	MET	2.8
1	B	59	ILE	2.8
1	B	151	PHE	2.7
1	B	327	PHE	2.7
1	A	228	TRP	2.7
1	B	457	VAL	2.7
1	B	363	HIS	2.7
1	B	11	SER	2.7
1	C	155	TRP	2.6
1	B	479	LYS	2.6
1	B	162	HIS	2.6
1	B	98	MET	2.6
1	B	428	LEU	2.6
1	B	299	LEU	2.6
1	A	156	GLY	2.6
1	C	157	GLU	2.6
1	B	43	ARG	2.6
1	B	369	LEU	2.6
1	B	391	VAL	2.6
1	B	239	ARG	2.5
1	B	267	VAL	2.5
1	B	360	ILE	2.5
1	B	373	GLN	2.5
1	B	292	PHE	2.5
1	B	411	ASN	2.5
1	B	436	LEU	2.5
1	B	100	ASN	2.4
1	B	520	MET	2.4
1	B	421	GLY	2.4
1	B	20	TRP	2.4
1	B	305	THR	2.4
1	B	313	GLN	2.4
1	B	425	HIS	2.4
1	B	268	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	365	HIS	2.4
1	B	126	LEU	2.4
1	B	213	LEU	2.4
1	B	459	THR	2.4
1	B	142	MET	2.3
1	B	210	MET	2.3
1	B	21	ASN	2.3
1	B	56	SER	2.3
1	B	286	GLY	2.3
1	B	108	TRP	2.3
1	B	189	LEU	2.3
1	B	346	LEU	2.3
1	B	258	THR	2.3
1	B	364	LEU	2.3
1	B	410	THR	2.3
1	B	322	TRP	2.3
1	B	273	LEU	2.3
1	B	435	THR	2.2
1	B	385	TYR	2.2
1	B	150	ARG	2.2
1	B	234	VAL	2.2
1	B	45	LEU	2.2
1	B	195	GLU	2.2
1	C	142	MET	2.2
1	B	475	TRP	2.2
1	B	222	VAL	2.2
1	A	155	TRP	2.2
1	B	357	ASP	2.2
1	B	366	GLY	2.2
1	B	218	LEU	2.2
1	B	416	ALA	2.2
1	B	221	THR	2.2
1	B	383	GLU	2.2
1	B	358	GLN	2.1
1	B	156	GLY	2.1
1	B	375	ASP	2.1
1	B	103	HIS	2.1
1	B	274	LEU	2.1
1	B	390	ASP	2.1
1	B	450	ALA	2.1
1	A	108	TRP	2.1
1	B	244	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	251	THR	2.1
1	B	386	GLU	2.1
1	A	512	THR	2.1
1	B	197	ALA	2.1
1	B	347	ILE	2.1
1	B	169	LEU	2.1
1	B	524	THR	2.1
1	B	165	PHE	2.1
1	B	379	LEU	2.1
1	B	50	ALA	2.1
1	B	174	TYR	2.1
1	B	380	ALA	2.1
1	B	412	ALA	2.0
1	B	362	LEU	2.0
1	B	106	TRP	2.0
1	B	422	ALA	2.0
1	B	54	TYR	2.0
1	A	162	HIS	2.0
1	B	83	VAL	2.0
1	B	198	THR	2.0
1	C	185	THR	2.0
1	B	295	LEU	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 monosaccharides 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.