



Full wwPDB X-ray Structure Validation Report i

Aug 9, 2020 – 10:23 AM BST

PDB ID : 7C3M
Title : Structure of FERM protein
Authors : Bu, W.; Loh, Z.Y.; Jin, S.; Basu, S.; Ero, R.; Park, J.E.; Yan, X.; Wang, M.; Sze, S.K.; Tan, S.M.; Gao, Y.G.
Deposited on : 2020-05-13
Resolution : 3.60 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 i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

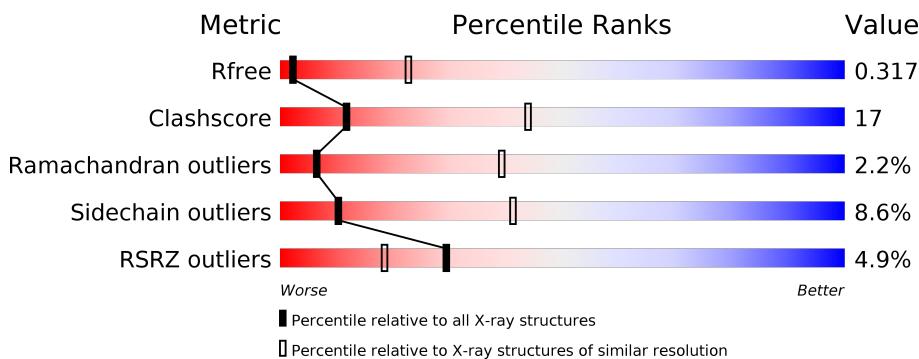
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

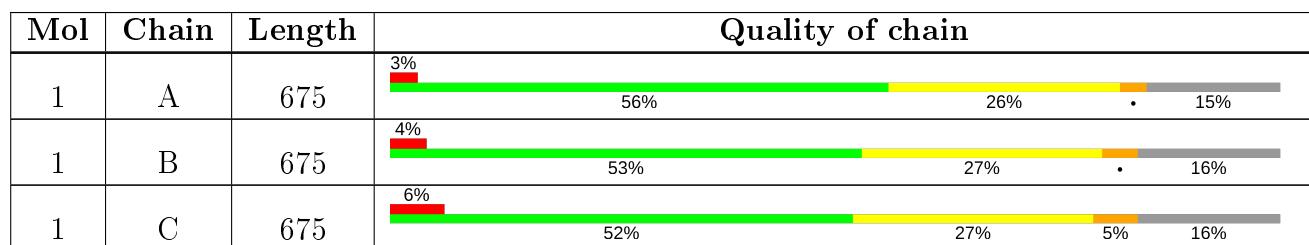
The reported resolution of this entry is 3.60 Å.

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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. 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.



2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 13538 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 Fermitin family homolog 3,Fermitin family homolog 3,Fermitin family homolog 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C 4575	N 2909	O 825	S 824	17	0	0
1	B	570	Total	C 4473	N 2837	O 805	S 811	20	0	0
1	C	570	Total	C 4490	N 2852	O 807	S 811	20	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	LEU	-	expression tag	UNP Q86UX7
A	669	GLU	-	expression tag	UNP Q86UX7
A	670	HIS	-	expression tag	UNP Q86UX7
A	671	HIS	-	expression tag	UNP Q86UX7
A	672	HIS	-	expression tag	UNP Q86UX7
A	673	HIS	-	expression tag	UNP Q86UX7
A	674	HIS	-	expression tag	UNP Q86UX7
A	675	HIS	-	expression tag	UNP Q86UX7
B	668	LEU	-	expression tag	UNP Q86UX7
B	669	GLU	-	expression tag	UNP Q86UX7
B	670	HIS	-	expression tag	UNP Q86UX7
B	671	HIS	-	expression tag	UNP Q86UX7
B	672	HIS	-	expression tag	UNP Q86UX7
B	673	HIS	-	expression tag	UNP Q86UX7
B	674	HIS	-	expression tag	UNP Q86UX7
B	675	HIS	-	expression tag	UNP Q86UX7
C	668	LEU	-	expression tag	UNP Q86UX7
C	669	GLU	-	expression tag	UNP Q86UX7
C	670	HIS	-	expression tag	UNP Q86UX7
C	671	HIS	-	expression tag	UNP Q86UX7
C	672	HIS	-	expression tag	UNP Q86UX7
C	673	HIS	-	expression tag	UNP Q86UX7

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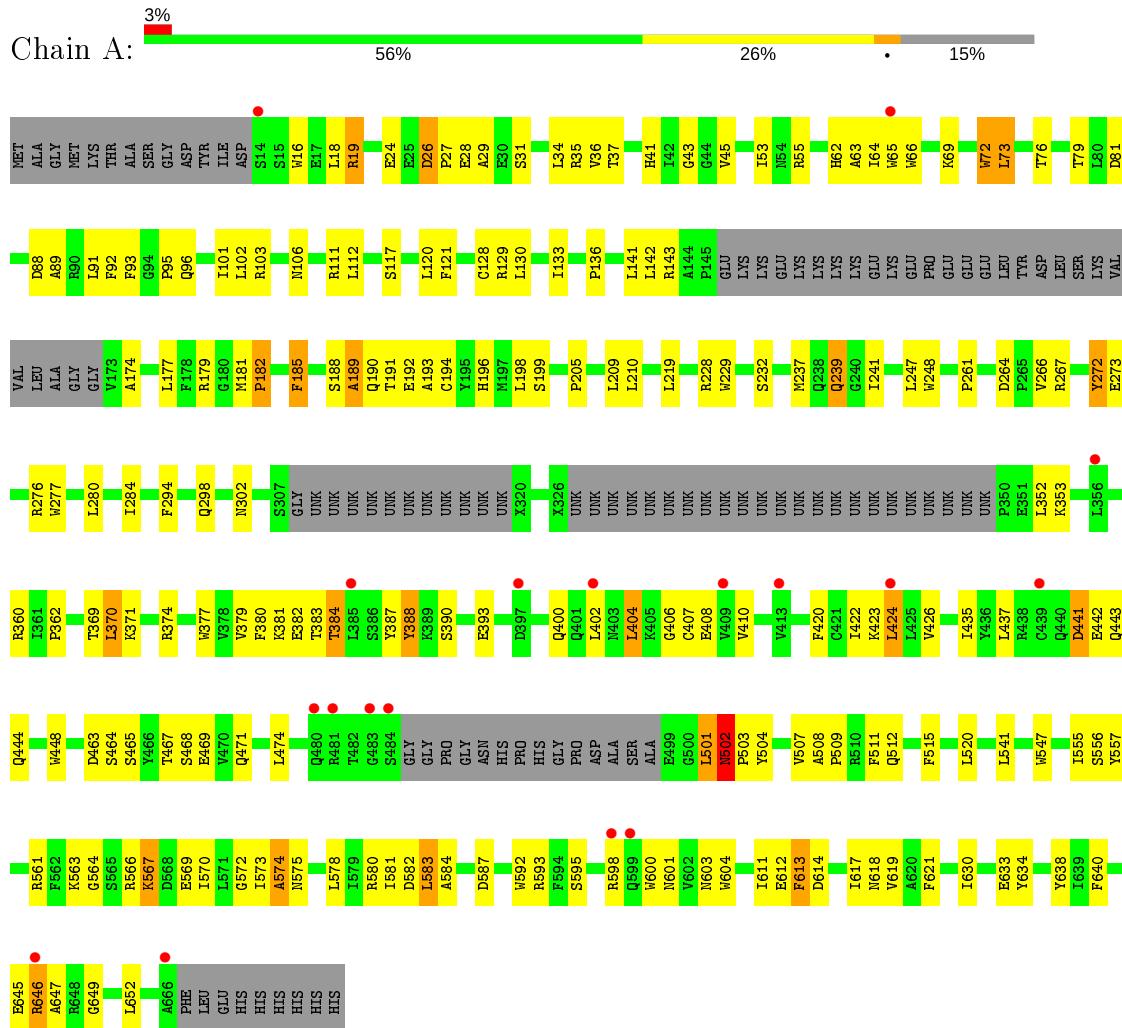
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Chain	Residue	Modelled	Actual	Comment	Reference
C	674	HIS	-	expression tag	UNP Q86UX7
C	675	HIS	-	expression tag	UNP Q86UX7

3 Residue-property plots [\(i\)](#)

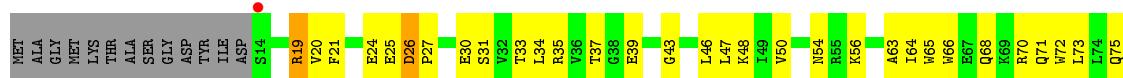
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

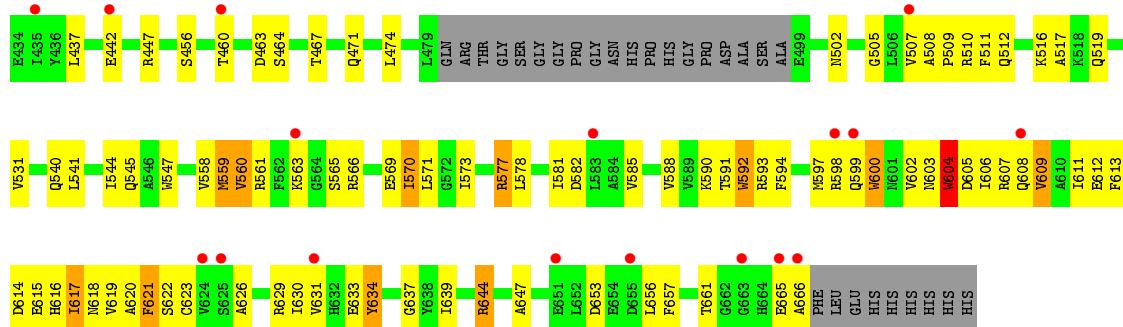
- Molecule 1: Fermitin family homolog 3,Fermitin family homolog 3,Fermitin family homolog 3



- Molecule 1: Fermitin family homolog 3,Fermitin family homolog 3,Fermitin family homolog 3







4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	115.76 Å 204.62 Å 269.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.60 49.20 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.20-3.60) 100.0 (49.20-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.10 (at 3.57 Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R , R_{free}	0.305 , 0.317 0.305 , 0.317	Depositor DCC
R_{free} test set	1771 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	170.3	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 140.3	EDS
L-test for twinning ²	$< L > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.034 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.038 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13538	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	0.27	0/4648	0.54	1/6306 (0.0%)
1	B	0.30	0/4537	0.56	0/6157
1	C	0.28	0/4571	0.55	0/6202
All	All	0.28	0/13756	0.55	1/18665 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
1	C	0	4
All	All	0	10

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	501	LEU	C-N-CA	5.53	135.52	121.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	603	ASN	Peptide
1	B	324	UNK	Peptide
1	B	363	ARG	Peptide
1	B	564	GLY	Peptide
1	B	595	SER	Peptide
1	B	612	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	104	LEU	Peptide
1	C	228	ARG	Peptide
1	C	287	THR	Peptide
1	C	366	ARG	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4575	0	4424	132	0
1	B	4473	0	4275	159	0
1	C	4490	0	4317	172	0
All	All	13538	0	13016	463	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 17.

All (463) 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:181:MET:HB3	1:B:182:PRO:HD2	1.50	0.92
1:C:104:LEU:HB2	1:C:106:ASN:H	1.33	0.92
1:B:600:TRP:HB3	1:B:611:ILE:HG23	1.52	0.89
1:C:360:ARG:HD3	1:C:361:ILE:H	1.39	0.88
1:A:120:LEU:HB3	1:A:232:SER:HA	1.55	0.88
1:B:292:MET:N	1:B:292:MET:SD	2.48	0.85
1:B:599:GLN:HG2	1:B:612:GLU:HB2	1.59	0.85
1:C:99:PRO:HD2	1:C:114:ALA:H	1.41	0.85
1:C:120:LEU:HB3	1:C:232:SER:HA	1.59	0.84
1:B:573:ILE:HA	1:B:578:LEU:HA	1.58	0.83
1:B:20:VAL:HG12	1:B:35:ARG:HG2	1.61	0.83
1:A:384:THR:HA	1:A:404:LEU:HD11	1.61	0.82
1:B:227:SER:HA	1:B:626:ALA:HB2	1.60	0.82
1:B:556:SER:OG	1:B:573:ILE:O	1.98	0.80
1:C:129:ARG:HH12	1:C:179:ARG:HB2	1.44	0.79
1:B:560:VAL:HA	1:B:623:CYS:SG	2.23	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ARG:HG2	1:C:104:LEU:HG	1.64	0.79
1:C:559:MET:HA	1:C:570:ILE:HA	1.66	0.78
1:A:64:ILE:HB	1:A:73:LEU:HD11	1.67	0.78
1:A:557:TYR:H	1:A:572:GLY:HA2	1.48	0.77
1:A:179:ARG:NH1	1:A:189:ALA:O	2.16	0.76
1:A:555:ILE:HD13	1:A:574:ALA:HB2	1.67	0.76
1:C:516:LYS:H	1:C:519:GLN:HE22	1.33	0.76
1:B:215:ARG:HE	1:B:509:PRO:HG3	1.50	0.76
1:B:569:GLU:OE2	1:B:580:ARG:NH2	2.19	0.76
1:C:142:LEU:HG	1:C:248:TRP:HB2	1.66	0.75
1:B:129:ARG:HH22	1:B:179:ARG:HB3	1.51	0.75
1:B:261:PRO:HB2	1:B:537:ALA:HB1	1.67	0.75
1:B:25:GLU:HB2	1:B:31:SER:HB2	1.69	0.74
1:B:217:SER:HB3	1:B:221:ASP:HB2	1.71	0.72
1:A:264:ASP:HB3	1:A:267:ARG:HB3	1.70	0.72
1:A:360:ARG:HB3	1:A:370:LEU:HD11	1.72	0.71
1:A:65:TRP:HB2	1:A:92:PHE:HB2	1.71	0.71
1:C:559:MET:HG3	1:C:626:ALA:HB2	1.72	0.71
1:A:383:THR:HG22	1:A:404:LEU:HD13	1.73	0.71
1:C:103:ARG:HG2	1:C:104:LEU:H	1.54	0.71
1:C:25:GLU:HB3	1:C:31:SER:HB2	1.72	0.71
1:A:72:TRP:CZ2	1:A:117:SER:HA	2.26	0.71
1:C:206:ASP:OD2	1:C:206:ASP:N	2.17	0.70
1:C:102:LEU:HD22	1:C:112:LEU:HD21	1.72	0.70
1:A:646:ARG:H	1:A:646:ARG:HD3	1.56	0.70
1:C:59:TRP:HE3	1:C:62:HIS:HE1	1.38	0.70
1:A:53:ILE:O	1:A:55:ARG:NH1	2.23	0.70
1:B:598:ARG:HB2	1:B:612:GLU:HG2	1.74	0.70
1:B:129:ARG:HH12	1:B:179:ARG:HB2	1.54	0.70
1:C:410:VAL:HB	1:C:423:LYS:HB3	1.74	0.70
1:C:103:ARG:HD3	1:C:248:TRP:CD1	2.25	0.70
1:C:581:ILE:HD12	1:C:582:ASP:H	1.57	0.70
1:B:368:LEU:HD13	1:B:369:THR:HG22	1.75	0.69
1:B:463:ASP:N	1:B:463:ASP:OD2	2.25	0.69
1:B:618:ASN:N	1:B:618:ASN:OD1	2.26	0.67
1:B:73:LEU:HD22	1:B:75:GLN:HE22	1.58	0.67
1:B:572:GLY:O	1:B:579:ILE:N	2.23	0.67
1:C:106:ASN:ND2	1:C:108:ARG:HE	1.93	0.67
1:C:402:LEU:HB2	1:C:426:VAL:HG11	1.76	0.66
1:C:560:VAL:HG23	1:C:569:GLU:HB3	1.77	0.66
1:B:561:ARG:N	1:B:623:CYS:HB3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:GLN:O	1:C:215:ARG:NH2	2.28	0.66
1:B:577:ARG:NH2	1:B:594:PHE:O	2.24	0.66
1:C:614:ASP:HB3	1:C:617:ILE:HG12	1.77	0.66
1:B:325:UNK:O	1:B:453:ARG:NH2	2.29	0.66
1:A:219:LEU:HD23	1:A:570:ILE:HD12	1.77	0.65
1:A:600:TRP:HB3	1:A:611:ILE:HA	1.78	0.65
1:B:599:GLN:O	1:B:612:GLU:N	2.29	0.65
1:C:73:LEU:O	1:C:75:GLN:N	2.29	0.65
1:A:567:LYS:HE3	1:A:583:LEU:HB3	1.78	0.65
1:C:623:CYS:HB3	1:C:626:ALA:HB3	1.78	0.65
1:A:102:LEU:HD22	1:A:112:LEU:HD21	1.78	0.65
1:A:142:LEU:HB3	1:A:248:TRP:HB2	1.78	0.65
1:C:34:LEU:HD11	1:C:48:LYS:HB3	1.79	0.64
1:C:598:ARG:NH2	1:C:615:GLU:OE2	2.31	0.63
1:C:603:ASN:ND2	1:C:608:GLN:O	2.31	0.63
1:B:215:ARG:HB2	1:B:281:LEU:O	1.97	0.63
1:B:35:ARG:O	1:B:48:LYS:NZ	2.24	0.63
1:B:98:ARG:HD3	1:B:243:ALA:HB2	1.80	0.63
1:C:108:ARG:NH1	1:C:197:MET:HB2	2.13	0.63
1:A:66:TRP:CZ3	1:A:89:ALA:HB3	2.35	0.62
1:A:402:LEU:HD13	1:A:426:VAL:HG21	1.82	0.62
1:C:101:ILE:HA	1:C:111:ARG:HA	1.82	0.62
1:A:188:SER:O	1:A:190:GLN:N	2.33	0.62
1:C:103:ARG:HG2	1:C:104:LEU:N	2.14	0.62
1:A:143:ARG:O	1:A:228:ARG:NH1	2.28	0.61
1:C:295:ALA:HB2	1:C:507:VAL:HG13	1.81	0.61
1:C:120:LEU:HD11	1:C:141:LEU:HD12	1.81	0.61
1:B:190:GLN:HE22	1:B:195:TYR:HB3	1.64	0.61
1:C:181:MET:HG3	1:C:369:THR:HA	1.81	0.61
1:C:600:TRP:HB3	1:C:611:ILE:HG22	1.82	0.61
1:C:104:LEU:HB3	1:C:108:ARG:O	2.00	0.61
1:A:272:TYR:CZ	1:A:276:ARG:HD2	2.36	0.61
1:B:120:LEU:HB3	1:B:232:SER:HA	1.82	0.61
1:C:581:ILE:HD13	1:C:588:VAL:H	1.65	0.61
1:B:358:ILE:HD11	1:B:378:VAL:HG22	1.83	0.60
1:A:141:LEU:HD13	1:A:247:LEU:HD13	1.82	0.60
1:B:99:PRO:HA	1:B:113:ARG:HA	1.83	0.60
1:C:99:PRO:CD	1:C:114:ALA:H	2.13	0.60
1:A:18:LEU:HD23	1:A:18:LEU:H	1.64	0.60
1:A:371:LYS:HD3	1:A:374:ARG:HH21	1.66	0.60
1:A:578:LEU:HD21	1:A:613:PHE:HZ	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:HIS:CE1	1:B:618:ASN:HD21	2.19	0.60
1:A:645:GLU:HB3	1:A:649:GLY:HA2	1.84	0.60
1:C:352:LEU:HD21	1:C:447:ARG:HE	1.67	0.60
1:C:597:MET:SD	1:C:600:TRP:NE1	2.74	0.60
1:C:463:ASP:OD1	1:C:464:SER:N	2.35	0.60
1:A:441:ASP:N	1:A:441:ASP:OD1	2.36	0.59
1:C:112:LEU:HA	1:C:175:PRO:HG3	1.83	0.59
1:B:410:VAL:HG23	1:B:423:LYS:HD3	1.83	0.59
1:A:502:ASN:HB2	1:A:503:PRO:HD2	1.83	0.59
1:C:360:ARG:HD3	1:C:361:ILE:N	2.14	0.59
1:C:573:ILE:HG21	1:C:634:TYR:HB3	1.85	0.59
1:C:360:ARG:NH2	1:C:400:GLN:OE1	2.36	0.59
1:B:412:ASP:HB2	1:B:423:LYS:HZ3	1.67	0.59
1:C:143:ARG:HD3	1:C:241:ILE:HD11	1.84	0.59
1:A:569:GLU:OE2	1:A:580:ARG:NH1	2.36	0.58
1:B:560:VAL:HG12	1:B:569:GLU:O	2.04	0.58
1:A:63:ALA:HB2	1:A:96:GLN:HE21	1.69	0.58
1:A:592:TRP:CE2	1:A:619:VAL:HG11	2.38	0.58
1:C:142:LEU:HB2	1:C:228:ARG:HD3	1.86	0.58
1:C:143:ARG:HG3	1:C:144:ALA:H	1.67	0.58
1:B:627:SER:O	1:B:630:ILE:N	2.32	0.58
1:C:130:LEU:HD12	1:C:179:ARG:HE	1.68	0.57
1:A:284:ILE:HG21	1:A:547:TRP:HE1	1.69	0.57
1:B:602:VAL:HG22	1:B:609:VAL:HG12	1.86	0.57
1:B:205:PRO:HB3	1:B:277:TRP:HH2	1.69	0.57
1:B:412:ASP:HB3	1:B:421:CYS:HB3	1.85	0.57
1:C:599:GLN:NE2	1:C:612:GLU:OE1	2.38	0.56
1:B:577:ARG:NH1	1:B:597:MET:SD	2.79	0.56
1:C:98:ARG:NH2	1:C:99:PRO:O	2.39	0.56
1:A:185:PHE:O	1:A:185:PHE:HD1	1.88	0.56
1:B:95:PRO:O	1:B:98:ARG:NH1	2.39	0.56
1:C:422:ILE:HG13	1:C:437:LEU:HB2	1.88	0.56
1:B:101:ILE:HG23	1:B:246:ALA:HA	1.88	0.56
1:B:577:ARG:HG3	1:B:592:TRP:HB2	1.88	0.56
1:B:531:VAL:HG13	1:B:534:LEU:HD12	1.88	0.56
1:B:66:TRP:CZ3	1:B:85:ILE:HG12	2.40	0.56
1:A:261:PRO:HG3	1:A:541:LEU:HD22	1.87	0.55
1:B:362:PRO:HG2	1:B:364:ARG:O	2.06	0.55
1:A:232:SER:OG	1:A:633:GLU:OE2	2.16	0.55
1:C:609:VAL:HG13	1:C:621:PHE:HE1	1.70	0.55
1:A:192:GLU:CD	1:A:193:ALA:H	2.11	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD11	1:A:280:LEU:HB3	1.89	0.55
1:C:573:ILE:HD11	1:C:631:VAL:HG23	1.87	0.55
1:B:535:SER:O	1:B:537:ALA:N	2.40	0.54
1:A:557:TYR:N	1:A:572:GLY:HA2	2.18	0.54
1:A:646:ARG:HG2	1:A:647:ALA:H	1.72	0.54
1:C:615:GLU:O	1:C:616:HIS:ND1	2.41	0.54
1:B:650:GLU:HG2	1:B:650:GLU:O	2.08	0.54
1:C:405:LYS:HA	1:C:456:SER:HA	1.89	0.54
1:B:64:ILE:HB	1:B:73:LEU:HB2	1.90	0.53
1:B:181:MET:HB3	1:B:182:PRO:CD	2.29	0.53
1:B:190:GLN:NE2	1:B:195:TYR:HB3	2.23	0.53
1:A:24:GLU:O	1:A:93:PHE:HB3	2.06	0.53
1:C:297:LEU:HD11	1:C:531:VAL:HG11	1.90	0.53
1:B:19:ARG:HD3	1:B:21:PHE:CZ	2.43	0.53
1:C:592:TRP:O	1:C:594:PHE:N	2.42	0.53
1:A:34:LEU:HD11	1:A:45:VAL:HG13	1.89	0.53
1:C:106:ASN:HD22	1:C:108:ARG:HE	1.54	0.53
1:C:226:HIS:HA	1:C:229:TRP:HE1	1.74	0.53
1:C:603:ASN:O	1:C:605:ASP:N	2.41	0.53
1:A:463:ASP:OD1	1:A:464:SER:N	2.42	0.53
1:C:100:VAL:HG11	1:C:245:ASP:HB2	1.91	0.53
1:C:104:LEU:HD13	1:C:106:ASN:O	2.09	0.53
1:A:181:MET:HA	1:A:369:THR:HG23	1.91	0.52
1:B:357:ARG:HE	1:B:373:TYR:HB3	1.73	0.52
1:C:607:ARG:NH1	1:C:623:CYS:O	2.42	0.52
1:B:580:ARG:HB2	1:B:592:TRP:HE1	1.74	0.52
1:B:352:LEU:HD21	1:B:447:ARG:HE	1.74	0.52
1:C:104:LEU:HB2	1:C:106:ASN:N	2.14	0.52
1:C:259:LEU:HB3	1:C:541:LEU:HD11	1.91	0.52
1:C:273:GLU:HG3	1:C:276:ARG:HD3	1.92	0.52
1:A:34:LEU:HD23	1:A:34:LEU:H	1.75	0.52
1:B:205:PRO:HB3	1:B:277:TRP:CH2	2.45	0.52
1:A:43:GLY:N	1:A:76:THR:O	2.43	0.52
1:A:179:ARG:NH2	1:A:190:GLN:HG2	2.24	0.52
1:A:567:LYS:NZ	1:A:582:ASP:OD1	2.39	0.52
1:B:129:ARG:NH2	1:B:181:MET:O	2.36	0.52
1:B:70:ARG:HB3	1:B:238:GLN:HG3	1.92	0.52
1:A:120:LEU:HD11	1:A:141:LEU:HD12	1.92	0.51
1:B:593:ARG:HB3	1:B:596:ASN:HD21	1.74	0.51
1:C:100:VAL:HB	1:C:245:ASP:O	2.10	0.51
1:C:62:HIS:HB3	1:C:96:GLN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:HG22	1:B:141:LEU:HG	1.91	0.51
1:B:410:VAL:HG23	1:B:423:LYS:HB2	1.91	0.51
1:B:534:LEU:HD13	1:B:542:ARG:HD3	1.92	0.51
1:C:73:LEU:O	1:C:75:GLN:HG2	2.11	0.51
1:B:562:PHE:HD2	1:B:569:GLU:OE1	1.93	0.51
1:C:24:GLU:HG2	1:C:92:PHE:CD1	2.45	0.51
1:C:99:PRO:HG2	1:C:114:ALA:HB3	1.92	0.51
1:A:598:ARG:HB2	1:A:612:GLU:HB3	1.93	0.51
1:C:223:THR:HB	1:C:558:VAL:O	2.10	0.51
1:A:569:GLU:HG3	1:A:580:ARG:HD2	1.93	0.51
1:A:66:TRP:NE1	1:A:69:LYS:HB3	2.26	0.51
1:B:186:SER:OG	1:B:423:LYS:NZ	2.20	0.51
1:B:611:ILE:H	1:B:619:VAL:CB	2.23	0.51
1:C:359:PHE:HD1	1:C:360:ARG:N	2.08	0.51
1:A:181:MET:HB2	1:A:182:PRO:HD2	1.92	0.51
1:B:561:ARG:NH2	1:B:567:LYS:HD2	2.25	0.51
1:A:613:PHE:HB2	1:A:617:ILE:O	2.10	0.51
1:A:407:CYS:SG	1:A:408:GLU:N	2.80	0.51
1:B:106:ASN:O	1:B:277:TRP:NE1	2.44	0.51
1:C:402:LEU:HD13	1:C:426:VAL:HG21	1.91	0.50
1:C:581:ILE:HD13	1:C:588:VAL:N	2.26	0.50
1:B:188:SER:O	1:B:190:GLN:HG2	2.10	0.50
1:B:231:ASP:N	1:B:231:ASP:OD1	2.45	0.50
1:B:291:MET:HA	1:B:294:PHE:HB2	1.92	0.50
1:C:301:ILE:HD12	1:C:540:GLN:HG3	1.93	0.50
1:B:34:LEU:H	1:B:34:LEU:HD23	1.75	0.50
1:C:39:GLU:OE1	1:C:39:GLU:N	2.44	0.50
1:B:611:ILE:HB	1:B:613:PHE:CE2	2.46	0.50
1:A:79:THR:HG22	1:A:81:ASP:H	1.77	0.50
1:A:575:ASN:HA	1:A:638:TYR:CG	2.46	0.50
1:B:19:ARG:H	1:B:19:ARG:HD2	1.77	0.50
1:A:501:LEU:O	1:A:502:ASN:O	2.30	0.50
1:B:278:ASP:O	1:B:283:GLU:HB3	2.12	0.50
1:B:444:GLN:O	1:B:448:TRP:HD1	1.95	0.50
1:C:100:VAL:HG22	1:C:247:LEU:HG	1.94	0.49
1:B:597:MET:HB3	1:B:600:TRP:HZ3	1.78	0.49
1:B:216:PRO:O	1:B:217:SER:HB2	2.13	0.49
1:C:420:PHE:CZ	1:C:442:GLU:HG3	2.48	0.49
1:C:573:ILE:HA	1:C:578:LEU:HD12	1.94	0.49
1:B:578:LEU:H	1:B:578:LEU:HD23	1.78	0.49
1:C:559:MET:O	1:C:560:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LEU:HD11	1:B:280:LEU:HG	1.94	0.49
1:C:96:GLN:NE2	1:C:117:SER:OG	2.37	0.49
1:C:612:GLU:HG3	1:C:618:ASN:OD1	2.12	0.49
1:A:26:ASP:O	1:A:28:GLU:O	2.31	0.49
1:A:353:LYS:HG2	1:A:379:VAL:HG22	1.94	0.49
1:B:369:THR:OG1	1:B:370:LEU:O	2.30	0.49
1:B:598:ARG:HB2	1:B:612:GLU:CG	2.40	0.49
1:A:582:ASP:O	1:A:584:ALA:N	2.36	0.49
1:B:559:MET:O	1:B:623:CYS:SG	2.70	0.49
1:B:560:VAL:C	1:B:623:CYS:HB3	2.33	0.49
1:C:353:LYS:HB3	1:C:377:TRP:CH2	2.48	0.49
1:B:407:CYS:SG	1:B:426:VAL:HA	2.53	0.49
1:C:288:GLU:O	1:C:289:GLU:HB2	2.13	0.49
1:C:467:THR:O	1:C:471:GLN:HG2	2.13	0.48
1:C:600:TRP:CZ2	1:C:639:ILE:HG13	2.47	0.48
1:A:103:ARG:N	1:A:247:LEU:O	2.43	0.48
1:B:460:THR:OG1	1:B:461:MET:N	2.46	0.48
1:B:577:ARG:HH21	1:B:594:PHE:C	2.14	0.48
1:C:282:GLU:HG3	1:C:509:PRO:HD2	1.95	0.48
1:A:381:LYS:HG2	1:A:382:GLU:HG3	1.95	0.48
1:B:140:SER:HB3	1:B:252:LYS:HD2	1.96	0.48
1:A:174:ALA:HB2	1:A:194:CYS:SG	2.53	0.48
1:B:579:ILE:HD11	1:B:587:ASP:OD1	2.14	0.48
1:B:420:PHE:CZ	1:B:442:GLU:HG2	2.49	0.48
1:A:556:SER:HG	1:A:634:TYR:HE2	1.61	0.48
1:A:18:LEU:HB3	1:A:37:THR:HG22	1.96	0.48
1:B:227:SER:HA	1:B:626:ALA:CB	2.36	0.48
1:C:282:GLU:OE1	1:C:510:ARG:NH1	2.44	0.48
1:A:129:ARG:NH1	1:A:182:PRO:O	2.38	0.47
1:A:601:ASN:N	1:A:601:ASN:OD1	2.46	0.47
1:C:215:ARG:NE	1:C:509:PRO:HG3	2.28	0.47
1:C:66:TRP:HA	1:C:90:ARG:O	2.14	0.47
1:C:359:PHE:HD1	1:C:360:ARG:H	1.61	0.47
1:A:370:LEU:HD23	1:A:371:LYS:O	2.14	0.47
1:C:111:ARG:HG3	1:C:175:PRO:HD3	1.96	0.47
1:C:247:LEU:HA	1:C:248:TRP:HE3	1.78	0.47
1:C:291:MET:HG3	1:C:507:VAL:CG1	2.45	0.47
1:B:465:SER:HA	1:B:468:SER:HB3	1.95	0.47
1:B:608:GLN:OE1	1:B:622:SER:HB3	2.15	0.47
1:C:145:PRO:HD3	1:C:248:TRP:CZ2	2.50	0.47
1:C:425:LEU:HB3	1:C:432:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:CYS:HB3	1:B:196:HIS:ND1	2.30	0.47
1:B:264:ASP:N	1:B:264:ASP:OD1	2.48	0.47
1:C:142:LEU:HA	1:C:229:TRP:HA	1.96	0.47
1:A:128:CYS:HB3	1:A:133:ILE:HB	1.97	0.47
1:A:205:PRO:HG3	1:A:277:TRP:CH2	2.50	0.47
1:B:120:LEU:HD11	1:B:141:LEU:HD12	1.96	0.47
1:C:230:LEU:HD12	1:C:232:SER:H	1.80	0.47
1:A:435:ILE:HG22	1:A:437:LEU:HD12	1.97	0.47
1:B:480:GLN:HG3	1:B:480:GLN:O	2.15	0.47
1:C:573:ILE:HG12	1:C:578:LEU:HD11	1.97	0.47
1:C:62:HIS:HA	1:C:96:GLN:HB2	1.95	0.47
1:A:387:TYR:CE1	1:A:400:GLN:HB2	2.50	0.47
1:C:196:HIS:O	1:C:196:HIS:ND1	2.47	0.47
1:B:561:ARG:HH22	1:B:567:LYS:HD2	1.80	0.46
1:C:100:VAL:CG2	1:C:247:LEU:HG	2.45	0.46
1:A:640:PHE:HE1	1:A:652:LEU:HD13	1.78	0.46
1:B:369:THR:OG1	1:B:370:LEU:N	2.48	0.46
1:C:64:ILE:HG13	1:C:93:PHE:HD1	1.79	0.46
1:A:198:LEU:H	1:A:198:LEU:HD23	1.79	0.46
1:A:569:GLU:HB2	1:A:581:ILE:O	2.15	0.46
1:B:26:ASP:N	1:B:26:ASP:OD1	2.48	0.46
1:A:72:TRP:N	1:A:72:TRP:CD1	2.75	0.46
1:C:143:ARG:O	1:C:228:ARG:NE	2.37	0.46
1:C:143:ARG:HB3	1:C:228:ARG:HB3	1.96	0.46
1:A:352:LEU:HB2	1:A:380:PHE:HB3	1.97	0.46
1:B:105:PRO:HD3	1:B:249:LEU:O	2.16	0.46
1:B:223:THR:OG1	1:B:223:THR:O	2.33	0.46
1:C:644:ARG:HG2	1:C:644:ARG:H	1.60	0.46
1:B:25:GLU:CB	1:B:31:SER:HB2	2.42	0.46
1:C:18:LEU:HG	1:C:37:THR:HA	1.97	0.46
1:C:421:CYS:HA	1:C:437:LEU:O	2.16	0.46
1:B:561:ARG:HG3	1:B:623:CYS:HA	1.98	0.46
1:C:226:HIS:HA	1:C:229:TRP:NE1	2.31	0.46
1:C:291:MET:HG3	1:C:507:VAL:HG12	1.97	0.46
1:A:241:ILE:HD13	1:A:247:LEU:HD21	1.96	0.46
1:C:141:LEU:HD22	1:C:247:LEU:HD13	1.97	0.46
1:C:62:HIS:HB2	1:C:94:GLY:O	2.16	0.46
1:A:179:ARG:HH22	1:A:190:GLN:HG2	1.80	0.45
1:B:30:GLU:O	1:B:30:GLU:HG2	2.16	0.45
1:C:355:HIS:CE1	1:C:377:TRP:HB2	2.52	0.45
1:C:665:GLU:HG3	1:C:666:ALA:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLU:HB2	1:C:92:PHE:HA	1.98	0.45
1:A:504:TYR:O	1:A:507:VAL:HG22	2.16	0.45
1:C:508:ALA:HB1	1:C:509:PRO:HA	1.98	0.45
1:A:41:HIS:O	1:A:45:VAL:HG23	2.17	0.45
1:A:467:THR:O	1:A:471:GLN:HG3	2.17	0.45
1:C:230:LEU:HD13	1:C:231:ASP:H	1.80	0.45
1:B:606:ILE:HG13	1:B:608:GLN:HB2	1.98	0.45
1:A:509:PRO:HA	1:A:512:GLN:HG2	1.99	0.45
1:A:561:ARG:NH1	1:A:566:ARG:HA	2.32	0.45
1:B:286:CYS:SG	1:B:291:MET:HB2	2.57	0.45
1:B:404:LEU:HA	1:B:407:CYS:SG	2.56	0.45
1:B:560:VAL:HG13	1:B:561:ARG:N	2.32	0.45
1:B:600:TRP:HA	1:B:610:ALA:O	2.16	0.45
1:A:66:TRP:HE1	1:A:69:LYS:HB3	1.80	0.45
1:B:65:TRP:HB3	1:B:92:PHE:HB2	1.98	0.45
1:C:103:ARG:HH21	1:C:250:ARG:HB3	1.82	0.45
1:A:353:LYS:HB3	1:A:377:TRP:CH2	2.52	0.44
1:C:257:PHE:HZ	1:C:647:ALA:H	1.65	0.44
1:A:422:ILE:HG12	1:A:437:LEU:HB2	1.99	0.44
1:A:504:TYR:CB	1:A:520:LEU:HD11	2.47	0.44
1:A:561:ARG:O	1:A:621:PHE:HB2	2.17	0.44
1:B:24:GLU:HG2	1:B:91:LEU:O	2.17	0.44
1:C:47:LEU:HA	1:C:50:VAL:HG22	1.99	0.44
1:C:271:LEU:HD23	1:C:544:ILE:HD13	2.00	0.44
1:C:609:VAL:HG13	1:C:621:PHE:CE1	2.50	0.44
1:C:561:ARG:HG2	1:C:622:SER:H	1.82	0.44
1:A:377:TRP:N	1:A:388:TYR:O	2.48	0.44
1:C:112:LEU:HA	1:C:175:PRO:CG	2.48	0.44
1:B:75:GLN:O	1:B:75:GLN:HG2	2.17	0.44
1:C:112:LEU:HA	1:C:175:PRO:CB	2.47	0.44
1:A:600:TRP:HB2	1:A:612:GLU:HB2	1.99	0.44
1:C:142:LEU:HG	1:C:248:TRP:CB	2.41	0.44
1:A:106:ASN:HA	1:A:273:GLU:HG2	2.00	0.44
1:A:362:PRO:HD3	1:A:370:LEU:HD13	1.99	0.44
1:C:563:LYS:HD3	1:C:620:ALA:HB3	2.00	0.44
1:B:202:GLN:H	1:B:202:GLN:HG2	1.44	0.44
1:A:443:GLN:HG2	1:A:474:LEU:HD21	2.00	0.43
1:A:229:TRP:HB2	1:A:630:ILE:HG21	2.00	0.43
1:C:578:LEU:O	1:C:591:THR:HB	2.18	0.43
1:B:253:TYR:CE1	1:B:637:GLY:HA3	2.53	0.43
1:B:541:LEU:HD23	1:B:541:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:VAL:HG13	1:B:561:ARG:O	2.19	0.43
1:C:104:LEU:HG	1:C:104:LEU:H	1.36	0.43
1:C:352:LEU:HD12	1:C:380:PHE:HD2	1.83	0.43
1:C:44:GLY:O	1:C:48:LYS:HD3	2.18	0.43
1:C:560:VAL:N	1:C:569:GLU:O	2.44	0.43
1:A:88:ASP:N	1:A:88:ASP:OD1	2.48	0.43
1:B:143:ARG:HG2	1:B:228:ARG:HB2	1.99	0.43
1:C:120:LEU:HD22	1:C:230:LEU:HB3	2.00	0.43
1:A:111:ARG:O	1:A:174:ALA:O	2.36	0.43
1:A:19:ARG:HD2	1:A:36:VAL:O	2.18	0.43
1:A:239:GLN:HB3	1:A:239:GLN:HE21	1.57	0.43
1:A:404:LEU:H	1:A:404:LEU:HG	1.48	0.43
1:C:15:SER:O	1:C:16:TRP:HD1	2.01	0.43
1:A:420:PHE:CE1	1:A:442:GLU:HG3	2.53	0.43
1:B:199:SER:O	1:B:269:THR:OG1	2.30	0.43
1:B:441:ASP:HB2	1:B:444:GLN:H	1.83	0.43
1:C:103:ARG:CB	1:C:248:TRP:HA	2.48	0.43
1:A:587:ASP:OD1	1:A:587:ASP:N	2.46	0.43
1:B:284:ILE:HD13	1:B:555:ILE:HG12	2.01	0.43
1:B:422:ILE:HB	1:B:437:LEU:HB2	2.01	0.43
1:B:270:GLN:O	1:B:274:GLN:N	2.51	0.43
1:B:414:ASN:HB3	1:B:419:LYS:HB3	2.00	0.43
1:B:71:GLN:HE22	1:B:83:TYR:HE1	1.67	0.43
1:A:129:ARG:CZ	1:A:181:MET:O	2.67	0.43
1:B:215:ARG:HG2	1:B:216:PRO:HD3	2.01	0.43
1:B:37:THR:HG23	1:B:39:GLU:H	1.83	0.43
1:B:534:LEU:O	1:B:538:GLU:HB2	2.19	0.43
1:B:555:ILE:HG22	1:B:557:TYR:CD2	2.54	0.43
1:B:97:HIS:HA	1:B:114:ALA:O	2.19	0.43
1:A:410:VAL:HG23	1:A:423:LYS:HB3	2.01	0.42
1:B:577:ARG:HA	1:B:577:ARG:HD3	1.69	0.42
1:A:188:SER:O	1:A:190:GLN:HG3	2.20	0.42
1:A:273:GLU:HG3	1:A:276:ARG:HD3	2.01	0.42
1:A:511:PHE:O	1:A:515:PHE:HB2	2.20	0.42
1:C:581:ILE:CD1	1:C:582:ASP:H	2.29	0.42
1:C:184:HIS:HB3	1:C:359:PHE:CE2	2.54	0.42
1:A:444:GLN:O	1:A:448:TRP:HD1	2.02	0.42
1:C:103:ARG:NH2	1:C:250:ARG:HB3	2.35	0.42
1:C:59:TRP:O	1:C:61:ASP:N	2.47	0.42
1:C:66:TRP:HZ3	1:C:73:LEU:CB	2.32	0.42
1:A:501:LEU:HA	1:A:501:LEU:HD12	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ALA:HB1	1:A:509:PRO:HD2	2.01	0.42
1:C:505:GLY:C	1:C:507:VAL:H	2.22	0.42
1:C:653:ASP:OD2	1:C:656:LEU:HB2	2.20	0.42
1:B:253:TYR:HB2	1:B:641:LEU:HD22	2.02	0.42
1:C:295:ALA:HB2	1:C:507:VAL:CG1	2.48	0.42
1:B:596:ASN:ND2	1:B:596:ASN:N	2.67	0.42
1:C:176:ALA:H	1:C:177:LEU:HD12	1.84	0.42
1:A:404:LEU:C	1:A:406:GLY:N	2.72	0.42
1:A:422:ILE:HD11	1:A:437:LEU:HD22	2.02	0.42
1:A:640:PHE:HZ	1:A:652:LEU:HB3	1.85	0.42
1:B:26:ASP:HB2	1:B:27:PRO:HD3	2.02	0.42
1:C:234:ARG:HB2	1:C:239:GLN:NE2	2.34	0.42
1:C:235:CYS:SG	1:C:238:GLN:HG3	2.59	0.42
1:C:302:ASN:C	1:C:304:LEU:H	2.22	0.42
1:C:602:VAL:HG13	1:C:604:TRP:CD1	2.54	0.42
1:C:565:SER:OG	1:C:566:ARG:N	2.53	0.42
1:B:195:TYR:HB2	1:B:198:LEU:HD11	2.01	0.42
1:B:195:TYR:CD2	1:B:199:SER:HB3	2.55	0.42
1:B:600:TRP:HA	1:B:611:ILE:HA	2.01	0.42
1:C:259:LEU:HD13	1:C:259:LEU:HA	1.92	0.42
1:C:560:VAL:HB	1:C:621:PHE:HB2	2.02	0.42
1:A:199:SER:HB3	1:A:266:VAL:HG22	2.02	0.41
1:A:573:ILE:HG21	1:A:634:TYR:HB3	2.01	0.41
1:A:600:TRP:HZ3	1:A:618:ASN:HB2	1.84	0.41
1:A:62:HIS:HA	1:A:95:PRO:HA	2.02	0.41
1:A:64:ILE:O	1:A:72:TRP:HB3	2.20	0.41
1:B:509:PRO:O	1:B:513:ARG:HG3	2.20	0.41
1:B:66:TRP:CD1	1:B:66:TRP:C	2.94	0.41
1:B:616:HIS:CD2	1:B:618:ASN:OD1	2.73	0.41
1:C:633:GLU:O	1:C:637:GLY:N	2.48	0.41
1:C:98:ARG:N	1:C:99:PRO:HD3	2.35	0.41
1:B:600:TRP:HD1	1:B:632:HIS:CE1	2.37	0.41
1:A:563:LYS:HG3	1:A:564:GLY:H	1.84	0.41
1:C:264:ASP:N	1:C:264:ASP:OD1	2.53	0.41
1:C:516:LYS:H	1:C:519:GLN:NE2	2.09	0.41
1:A:130:LEU:HD12	1:A:179:ARG:HE	1.85	0.41
1:B:420:PHE:HZ	1:B:442:GLU:HG2	1.86	0.41
1:C:106:ASN:ND2	1:C:108:ARG:O	2.54	0.41
1:C:138:GLU:HA	1:C:253:TYR:HD2	1.85	0.41
1:C:560:VAL:CG2	1:C:571:LEU:HB2	2.51	0.41
1:A:128:CYS:HB2	1:A:136:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:SER:O	1:A:469:GLU:N	2.53	0.41
1:B:43:GLY:HA2	1:B:46:LEU:HD13	2.02	0.41
1:B:577:ARG:HD3	1:B:578:LEU:H	1.85	0.41
1:C:577:ARG:HB2	1:C:592:TRP:HA	2.02	0.41
1:A:390:SER:HB3	1:A:393:GLU:HG3	2.02	0.41
1:A:593:ARG:HG3	1:A:595:SER:H	1.85	0.41
1:B:353:LYS:HB2	1:B:377:TRP:CH2	2.55	0.41
1:B:578:LEU:HD21	1:B:613:PHE:CZ	2.56	0.41
1:C:31:SER:OG	1:C:32:VAL:HG23	2.21	0.41
1:C:594:PHE:HD1	1:C:639:ILE:HD11	1.86	0.41
1:C:629:ARG:HH12	1:C:661:THR:HG22	1.85	0.41
1:B:68:GLN:NE2	1:B:88:ASP:O	2.54	0.41
1:C:140:SER:HB3	1:C:252:LYS:HD2	2.03	0.41
1:C:25:GLU:HB3	1:C:31:SER:CB	2.46	0.41
1:C:597:MET:HA	1:C:613:PHE:O	2.21	0.41
1:C:615:GLU:O	1:C:617:ILE:HG23	2.21	0.41
1:A:29:ALA:HB1	1:A:92:PHE:HE2	1.86	0.41
1:B:597:MET:HB3	1:B:600:TRP:CZ3	2.56	0.41
1:B:75:GLN:HB2	1:B:78:TRP:CD1	2.56	0.41
1:B:535:SER:O	1:B:538:GLU:N	2.55	0.40
1:A:502:ASN:HD22	1:A:502:ASN:C	2.23	0.40
1:B:223:THR:CG2	1:B:559:MET:HG3	2.51	0.40
1:B:608:GLN:OE1	1:B:622:SER:CB	2.69	0.40
1:A:294:PHE:O	1:A:298:GLN:HG3	2.21	0.40
1:A:424:LEU:HD11	1:A:435:ILE:HB	2.04	0.40
1:B:63:ALA:HB3	1:B:72:TRP:HZ3	1.86	0.40
1:B:66:TRP:HZ3	1:B:85:ILE:HG12	1.83	0.40
1:C:512:GLN:HG3	1:C:517:ALA:HB2	2.04	0.40
1:B:294:PHE:HD2	1:B:543:PHE:CE1	2.38	0.40
1:B:412:ASP:OD2	1:B:419:LYS:HD3	2.21	0.40
1:B:47:LEU:HA	1:B:50:VAL:HG23	2.02	0.40
1:C:142:LEU:HD21	1:C:250:ARG:HG2	2.03	0.40
1:A:103:ARG:HG3	1:A:248:TRP:CE2	2.56	0.40
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.89	0.40
1:B:354:ASP:HB2	1:B:448:TRP:HZ2	1.86	0.40
1:C:234:ARG:HB2	1:C:239:GLN:HE21	1.86	0.40
1:C:545:GLN:C	1:C:547:TRP:H	2.24	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	562/675 (83%)	476 (85%)	76 (14%)	10 (2%)	8 43
1	B	554/675 (82%)	455 (82%)	82 (15%)	17 (3%)	4 32
1	C	557/675 (82%)	469 (84%)	78 (14%)	10 (2%)	8 43
All	All	1673/2025 (83%)	1400 (84%)	236 (14%)	37 (2%)	6 39

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	ASN
1	B	536	LEU
1	B	565	SER
1	B	594	PHE
1	B	595	SER
1	B	613	PHE
1	C	74	LEU
1	C	229	TRP
1	C	288	GLU
1	A	604	TRP
1	B	596	ASN
1	C	593	ARG
1	A	26	ASP
1	A	27	PRO
1	A	614	ASP
1	B	553	PHE
1	B	567	LYS
1	C	559	MET
1	A	574	ALA
1	B	363	ARG
1	B	614	ASP
1	C	181	MET
1	C	182	PRO
1	C	604	TRP

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Mol	Chain	Res	Type
1	A	189	ALA
1	A	583	LEU
1	B	56	LYS
1	B	361	ILE
1	B	362	PRO
1	B	535	SER
1	A	613	PHE
1	B	364	ARG
1	B	569	GLU
1	C	367	LYS
1	B	570	ILE
1	C	42	ILE
1	A	182	PRO

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	471/551 (86%)	443 (94%)	28 (6%)	19 55
1	B	455/551 (83%)	416 (91%)	39 (9%)	10 41
1	C	461/551 (84%)	409 (89%)	52 (11%)	6 30
All	All	1387/1653 (84%)	1268 (91%)	119 (9%)	10 41

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	TRP
1	A	19	ARG
1	A	31	SER
1	A	35	ARG
1	A	72	TRP
1	A	73	LEU
1	A	91	LEU
1	A	101	ILE
1	A	121	PHE

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Mol	Chain	Res	Type
1	A	177	LEU
1	A	185	PHE
1	A	191	THR
1	A	196	HIS
1	A	209	LEU
1	A	237	MET
1	A	239	GLN
1	A	272	TYR
1	A	302	ASN
1	A	370	LEU
1	A	384	THR
1	A	388	TYR
1	A	404	LEU
1	A	424	LEU
1	A	441	ASP
1	A	468	SER
1	A	502	ASN
1	A	567	LYS
1	A	646	ARG
1	B	19	ARG
1	B	26	ASP
1	B	33	THR
1	B	54	ASN
1	B	202	GLN
1	B	215	ARG
1	B	223	THR
1	B	239	GLN
1	B	258	ASP
1	B	268	LEU
1	B	278	ASP
1	B	280	LEU
1	B	285	ASP
1	B	292	MET
1	B	293	VAL
1	B	301	ILE
1	B	359	PHE
1	B	360	ARG
1	B	368	LEU
1	B	369	THR
1	B	380	PHE
1	B	402	LEU
1	B	463	ASP

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Mol	Chain	Res	Type
1	B	481	ARG
1	B	550	LEU
1	B	555	ILE
1	B	559	MET
1	B	560	VAL
1	B	569	GLU
1	B	577	ARG
1	B	579	ILE
1	B	591	THR
1	B	596	ASN
1	B	606	ILE
1	B	611	ILE
1	B	615	GLU
1	B	616	HIS
1	B	618	ASN
1	B	634	TYR
1	C	24	GLU
1	C	37	THR
1	C	48	LYS
1	C	74	LEU
1	C	98	ARG
1	C	104	LEU
1	C	106	ASN
1	C	108	ARG
1	C	116	PHE
1	C	131	LEU
1	C	142	LEU
1	C	185	PHE
1	C	188	SER
1	C	192	GLU
1	C	197	MET
1	C	206	ASP
1	C	228	ARG
1	C	230	LEU
1	C	239	GLN
1	C	248	TRP
1	C	250	ARG
1	C	273	GLU
1	C	286	CYS
1	C	289	GLU
1	C	291	MET
1	C	359	PHE

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Mol	Chain	Res	Type
1	C	360	ARG
1	C	373	TYR
1	C	374	ARG
1	C	402	LEU
1	C	422	ILE
1	C	460	THR
1	C	474	LEU
1	C	502	ASN
1	C	511	PHE
1	C	560	VAL
1	C	570	ILE
1	C	577	ARG
1	C	585	VAL
1	C	590	LYS
1	C	592	TRP
1	C	600	TRP
1	C	604	TRP
1	C	606	ILE
1	C	609	VAL
1	C	617	ILE
1	C	619	VAL
1	C	621	PHE
1	C	630	ILE
1	C	634	TYR
1	C	644	ARG
1	C	657	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	202	GLN
1	A	444	GLN
1	A	502	ASN
1	A	528	HIS
1	B	54	ASN
1	B	75	GLN
1	B	190	GLN
1	B	302	ASN
1	B	519	GLN
1	B	616	HIS
1	C	62	HIS

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Mol	Chain	Res	Type
1	C	106	ASN
1	C	596	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 [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	570/675 (84%)	0.30	18 (3%) 47 32	126, 154, 192, 224	0
1	B	562/675 (83%)	0.35	27 (4%) 30 19	143, 184, 225, 246	0
1	C	565/675 (83%)	0.46	38 (6%) 17 10	139, 179, 214, 227	0
All	All	1697/2025 (83%)	0.37	83 (4%) 29 18	126, 173, 215, 246	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	557	TYR	7.9
1	C	666	ALA	7.7
1	C	599	GLN	5.0
1	B	666	ALA	4.8
1	A	484	SER	4.8
1	B	480	GLN	4.7
1	A	666	ALA	4.4
1	B	14	SER	3.9
1	C	56	LYS	3.9
1	C	303	LYS	3.8
1	C	34	LEU	3.7
1	C	400	GLN	3.7
1	A	397	ASP	3.6
1	C	624	VAL	3.6
1	A	483	GLY	3.5
1	C	665	GLU	3.5
1	A	439	CYS	3.4
1	B	634	TYR	3.3
1	A	356	LEU	3.1
1	B	556	SER	3.1
1	C	433	SER	3.0
1	B	597	MET	3.0
1	C	402	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	184	HIS	3.0
1	C	399	ILE	2.9
1	C	401	GLN	2.9
1	B	399	ILE	2.9
1	C	460	THR	2.9
1	C	507	VAL	2.9
1	A	480	GLN	2.9
1	C	33	THR	2.8
1	B	452	CYS	2.8
1	B	93	PHE	2.8
1	C	663	GLY	2.7
1	C	625	SER	2.7
1	B	305	SER	2.7
1	A	599	GLN	2.7
1	C	651	GLU	2.6
1	C	380	PHE	2.6
1	B	219	LEU	2.6
1	C	598	ARG	2.6
1	B	201	PRO	2.6
1	B	210	LEU	2.6
1	A	598	ARG	2.5
1	C	31	SER	2.5
1	C	631	VAL	2.5
1	B	298	GLN	2.4
1	A	481	ARG	2.4
1	A	65	TRP	2.4
1	C	422	ILE	2.4
1	C	21	PHE	2.3
1	B	83	TYR	2.3
1	C	350	PRO	2.3
1	C	608	GLN	2.3
1	B	547	TRP	2.3
1	B	138	GLU	2.3
1	B	110	LEU	2.3
1	C	393	GLU	2.2
1	C	387	TYR	2.2
1	A	409	VAL	2.2
1	B	665	GLU	2.2
1	C	48	LYS	2.2
1	B	435	ILE	2.2
1	A	402	LEU	2.2
1	C	426	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	413	VAL	2.1
1	A	646	ARG	2.1
1	C	655	ASP	2.1
1	C	389	LYS	2.1
1	C	442	GLU	2.1
1	C	435	ILE	2.1
1	B	664	HIS	2.1
1	C	563	LYS	2.1
1	B	99	PRO	2.1
1	B	256	PHE	2.1
1	A	385	LEU	2.1
1	B	663	GLY	2.0
1	B	85	ILE	2.0
1	B	573	ILE	2.0
1	C	14	SER	2.0
1	A	14	SER	2.0
1	A	424	LEU	2.0
1	C	583	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.