



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:22 AM UTC

PDB ID : 7C3M / pdb_00007c3m
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 ⓘ 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

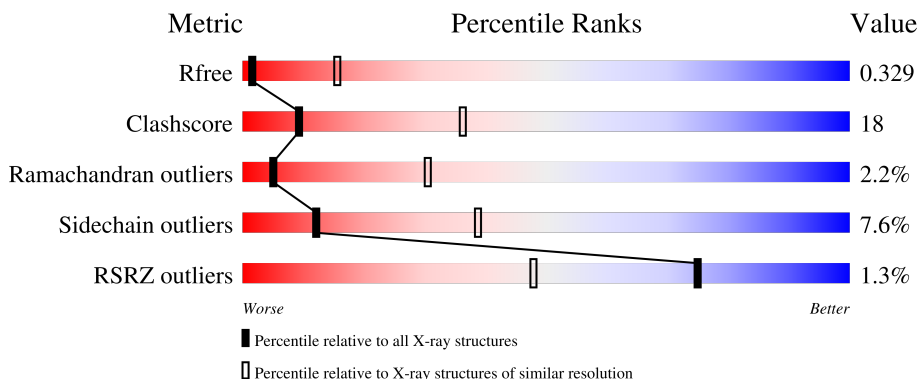
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (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 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	675	% 56% 27% • 15%
1	B	675	% 53% 27% • • 16%
1	C	675	% 52% 28% • • 16%

2 Entry composition

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	N	O	S	0	0	0
			4575	2909	825	824	17			
1	B	570	Total	C	N	O	S	0	0	0
			4473	2837	805	811	20			
1	C	570	Total	C	N	O	S	0	0	0
			4490	2852	807	811	20			

There are 24 discrepancies between the modelled and reference sequences:

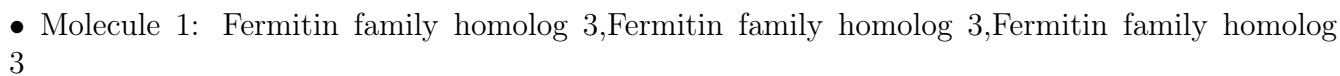
Chain	Residue	Modelled	Actual	Comment	Reference
A	668	LEU	-	expression tag	UNP Q86UX7
A	669	GLU	-	expression tag	UNP Q86UX7
A	670	HIS	-	expression tag	UNP Q86UX7
A	671	HIS	-	expression tag	UNP Q86UX7
A	672	HIS	-	expression tag	UNP Q86UX7
A	673	HIS	-	expression tag	UNP Q86UX7
A	674	HIS	-	expression tag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

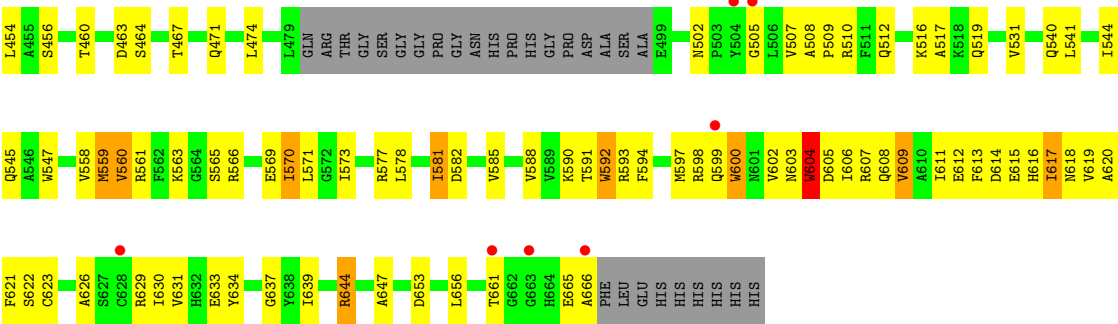
Continued on next page...

Continued from previous page...

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

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





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	115.76Å 204.62Å 269.95Å 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) 99.9 (49.20-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.305 , 0.317 0.311 , 0.329	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)	0.34 , 157.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	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	0.91	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.20	0/4648	0.57	6/6306 (0.1%)
1	B	0.24	0/4537	0.57	3/6157 (0.0%)
1	C	0.20	0/4571	0.56	2/6202 (0.0%)
All	All	0.21	0/13756	0.57	11/18665 (0.1%)

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 (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ASP	N-CA-C	-6.85	103.95	112.72
1	A	187	ASP	CA-C-N	5.97	130.47	121.40
1	A	187	ASP	C-N-CA	5.97	130.47	121.40
1	B	595	SER	CA-C-N	5.82	132.65	121.54
1	B	595	SER	C-N-CA	5.82	132.65	121.54
1	B	565	SER	N-CA-C	5.79	123.13	110.80
1	A	501	LEU	CA-C-N	5.62	135.52	121.80
1	A	501	LEU	C-N-CA	5.62	135.52	121.80
1	C	287	THR	CA-C-N	5.61	132.26	121.54
1	C	287	THR	C-N-CA	5.61	132.26	121.54
1	A	188	SER	N-CA-C	-5.10	98.62	107.49

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
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	135	0
1	B	4473	0	4275	169	0
1	C	4490	0	4317	177	0
All	All	13538	0	13016	481	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 18.

All (481) 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:SD	1:B:292:MET:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:72:TRP:H	1:A:72:TRP:CD1	2.01	0.77
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:186:SER:OG	1:B:423:LYS:NZ	2.20	0.73
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:25:GLU:HB3	1:C:31:SER:HB2	1.72	0.71
1:C:103:ARG:HG2	1:C:104:LEU:H	1.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:B:618:ASN:N	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
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:35:ARG:O	1:B:48:LYS:NZ	2.24	0.63
1:B:215:ARG:HB2	1:B:281:LEU:O	1.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:192:GLU:CD	1:A:193:ALA:H	2.11	0.59
1:A:441:ASP:OD1	1:A:441:ASP:N	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: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:B:16:TRP:H	1:B:16:TRP:CD1	2.22	0.56
1:C:98:ARG:NH2	1:C:99:PRO:O	2.39	0.56
1:A:185:PHE:HD1	1:A:185:PHE:O	1.88	0.56
1:B:95:PRO:O	1:B:98:ARG:NH1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:16:TRP:CG	1:B:17:GLU:H	2.25	0.54
1:B:650:GLU:O	1:B:650:GLU:HG2	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:560:VAL:C	1:B:623:CYS:HB3	2.33	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:B:577:ARG:HH21	1:B:594:PHE:C	2.14	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:352:LEU:HG	1:B:461:MET:HE1	1.92	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
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:66:TRP:NE1	1:A:69:LYS:HB3	2.26	0.51
1:A:569:GLU:HG3	1:A:580:ARG:HD2	1.93	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: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:OD1	1:B:231:ASP:N	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:N	1:C:39:GLU:OE1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:B:578:LEU:H	1.78	0.49
1:C:559:MET:O	1:C:560:VAL:HG13	2.12	0.49
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:C:353:LYS:HB3	1:C:377:TRP:CH2	2.48	0.49
1:A:407:CYS:SG	1:A:408:GLU:N	2.80	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: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:B:460:THR:OG1	1:B:461:MET:N	2.46	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: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:404:LEU:C	1:A:406:GLY:N	2.72	0.47
1:A:601:ASN:OD1	1:A:601:ASN:N	2.46	0.47
1:C:66:TRP:HA	1:C:90:ARG:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:NE	1:C:509:PRO:HG3	2.28	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
1:B:194:CYS:HB3	1:B:196:HIS:ND1	2.30	0.47
1:C:142:LEU:HA	1:C:229:TRP:HA	1.96	0.47
1:C:505:GLY:C	1:C:507:VAL:H	2.22	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:O	1:B:480:GLN:HG3	2.15	0.47
1:C:62:HIS:HA	1:C:96:GLN:HB2	1.95	0.47
1:C:302:ASN:C	1:C:304:LEU:H	2.22	0.47
1:C:573:ILE:HG12	1:C:578:LEU:HD11	1.97	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:OD1	1:B:26:ASP:N	2.48	0.46
1:A:72:TRP:CD1	1:A:72:TRP:N	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:O	1:B:223:THR:OG1	2.33	0.46
1:C:644:ARG:H	1:C:644:ARG:HG2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:CYS:HA	1:C:437:LEU:O	2.16	0.46
1:B:66:TRP:CD1	1:B:66:TRP:C	2.94	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:181:MET:HB2	1:A:181:MET:HE2	1.78	0.46
1:A:241:ILE:HD13	1:A:247:LEU:HD21	1.96	0.46
1:C:545:GLN:C	1:C:547:TRP:H	2.24	0.46
1:B:264:ASP:OD1	1:B:264:ASP:N	2.48	0.46
1:C:62:HIS:HB2	1:C:94:GLY:O	2.16	0.46
1:C:141:LEU:HD22	1:C:247:LEU:HD13	1.97	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:24:GLU:HB2	1:C:92:PHE:HA	1.98	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
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:A:502:ASN:C	1:A:502:ASN:HD22	2.23	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: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:B:565:SER:CB	1:B:569:GLU:CD	2.90	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:561:ARG:HG2	1:C:622:SER:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:609:VAL:HG13	1:C:621:PHE:CE1	2.50	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:73:LEU:O	1:C:74:LEU:C	2.61	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:229:TRP:HB2	1:A:630:ILE:HG21	2.00	0.43
1:A:443:GLN:HG2	1:A:474:LEU:HD21	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
1:B:560:VAL:HG13	1:B:561:ARG:O	2.19	0.43
1:C:44:GLY:O	1:C:48:LYS:HD3	2.18	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: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:19:ARG:HD2	1:A:36:VAL:O	2.18	0.43
1:A:111:ARG:O	1:A:174:ALA:O	2.36	0.43
1:A:239:GLN:HE21	1:A:239:GLN:HB3	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: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:560:VAL:HG13	1:B:561:ARG:N	2.32	0.43
1:B:71:GLN:HE22	1:B:83:TYR:HE1	1.67	0.43
1:B:270:GLN:O	1:B:274:GLN:N	2.51	0.43
1:B:291:MET:HE2	1:B:508:ALA:H	1.83	0.43
1:B:414:ASN:HB3	1:B:419:LYS:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:CZ	1:A:181:MET:O	2.67	0.43
1:B:37:THR:HG23	1:B:39:GLU:H	1.83	0.43
1:B:97:HIS:HA	1:B:114:ALA:O	2.19	0.43
1:B:215:ARG:HG2	1:B:216:PRO:HD3	2.01	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:A:410:VAL:HG23	1:A:423:LYS:HB3	2.01	0.42
1:B:577:ARG:HD3	1:B:577:ARG:HA	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:B:285:ASP:O	1:B:285:ASP:CG	2.63	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:C:103:ARG:NH2	1:C:250:ARG:HB3	2.35	0.42
1:A:501:LEU:HD12	1:A:501:LEU:HA	1.82	0.42
1:A:508:ALA:HB1	1:A:509:PRO:HD2	2.01	0.42
1:C:653:ASP:OD2	1:C:656:LEU:HB2	2.20	0.42
1:A:219:LEU:C	1:A:221:ASP:H	2.28	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: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: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:62:HIS:HA	1:A:95:PRO:HA	2.02	0.41
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:TRP:HZ3	1:A:618:ASN:HB2	1.84	0.41
1:B:562:PHE:HD2	1:B:569:GLU:CD	2.27	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:616:HIS:CD2	1:B:618:ASN:OD1	2.73	0.41
1:C:98:ARG:N	1:C:99:PRO:HD3	2.35	0.41
1:C:106:ASN:CG	1:C:108:ARG:HH21	2.29	0.41
1:C:110:LEU:HD22	1:C:197:MET:HE1	2.03	0.41
1:C:633:GLU:O	1:C:637:GLY:N	2.48	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:OD1	1:C:264:ASP:N	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
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:B:650:GLU:O	1:B:651:GLU:C	2.64	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:A:29:ALA:HB1	1:A:92:PHE:HE2	1.86	0.41
1:B:68:GLN:NE2	1:B:88:ASP:O	2.54	0.41
1:B:626:ALA:O	1:B:627:SER:C	2.64	0.41
1:C:25:GLU:HB3	1:C:31:SER:CB	2.46	0.41
1:C:75:GLN:C	1:C:77:HIS:H	2.29	0.41
1:C:140:SER:HB3	1:C:252:LYS:HD2	2.03	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:B:75:GLN:HB2	1:B:78:TRP:CD1	2.56	0.41
1:B:597:MET:HB3	1:B:600:TRP:CZ3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:SER:O	1:B:538:GLU:N	2.55	0.40
1:B:577:ARG:HG2	1:B:592:TRP:C	2.46	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:A:600:TRP:CD1	1:A:601:ASN:H	2.40	0.40
1:B:47:LEU:HA	1:B:50:VAL:HG23	2.02	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:C:142:LEU:HD21	1:C:250:ARG:HG2	2.03	0.40
1:C:181:MET:O	1:C:182:PRO:C	2.65	0.40
1:A:103:ARG:HG3	1:A:248:TRP:CE2	2.56	0.40
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.89	0.40
1:B:181:MET:O	1:B:182:PRO:C	2.65	0.40
1:B:354:ASP:HB2	1:B:448:TRP:HZ2	1.86	0.40
1:B:535:SER:C	1:B:537:ALA:N	2.79	0.40
1:C:234:ARG:HB2	1:C:239:GLN:HE21	1.86	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	562/675 (83%)	476 (85%)	76 (14%)	10 (2%)	6	34
1	B	554/675 (82%)	455 (82%)	82 (15%)	17 (3%)	3	25
1	C	557/675 (82%)	469 (84%)	78 (14%)	10 (2%)	6	34
All	All	1673/2025 (83%)	1400 (84%)	236 (14%)	37 (2%)	5	30

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
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 ⓘ

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%)	446 (95%)	25 (5%)	20	48
1	B	455/551 (83%)	420 (92%)	35 (8%)	12	38
1	C	461/551 (84%)	415 (90%)	46 (10%)	7	30
All	All	1387/1653 (84%)	1281 (92%)	106 (8%)	12	39

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	TRP
1	A	31	SER
1	A	35	ARG
1	A	47	LEU
1	A	72	TRP
1	A	73	LEU
1	A	91	LEU
1	A	101	ILE
1	A	177	LEU
1	A	185	PHE
1	A	191	THR
1	A	209	LEU
1	A	237	MET
1	A	239	GLN
1	A	301	ILE
1	A	370	LEU
1	A	384	THR
1	A	404	LEU
1	A	424	LEU
1	A	441	ASP
1	A	468	SER
1	A	501	LEU
1	A	502	ASN
1	A	523	ARG
1	A	619	VAL
1	B	19	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	26	ASP
1	B	33	THR
1	B	36	VAL
1	B	54	ASN
1	B	101	ILE
1	B	202	GLN
1	B	223	THR
1	B	239	GLN
1	B	268	LEU
1	B	278	ASP
1	B	280	LEU
1	B	284	ILE
1	B	285	ASP
1	B	292	MET
1	B	293	VAL
1	B	301	ILE
1	B	359	PHE
1	B	368	LEU
1	B	369	THR
1	B	402	LEU
1	B	463	ASP
1	B	481	ARG
1	B	550	LEU
1	B	555	ILE
1	B	560	VAL
1	B	569	GLU
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	C	24	GLU
1	C	36	VAL
1	C	37	THR
1	C	74	LEU
1	C	104	LEU
1	C	106	ASN
1	C	108	ARG
1	C	116	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	131	LEU
1	C	142	LEU
1	C	173	VAL
1	C	185	PHE
1	C	188	SER
1	C	192	GLU
1	C	206	ASP
1	C	228	ARG
1	C	230	LEU
1	C	239	GLN
1	C	248	TRP
1	C	249	LEU
1	C	250	ARG
1	C	266	VAL
1	C	273	GLU
1	C	289	GLU
1	C	360	ARG
1	C	399	ILE
1	C	402	LEU
1	C	422	ILE
1	C	454	LEU
1	C	460	THR
1	C	474	LEU
1	C	502	ASN
1	C	560	VAL
1	C	570	ILE
1	C	581	ILE
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	630	ILE
1	C	644	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	196	HIS
1	A	202	GLN
1	A	226	HIS
1	A	298	GLN
1	A	391	GLN
1	A	444	GLN
1	A	502	ASN
1	A	528	HIS
1	A	529	GLN
1	A	548	GLN
1	B	54	ASN
1	B	62	HIS
1	B	75	GLN
1	B	77	HIS
1	B	118	GLN
1	B	122	GLN
1	B	190	GLN
1	B	300	HIS
1	B	519	GLN
1	B	528	HIS
1	B	601	ASN
1	B	616	HIS
1	B	659	GLN
1	C	57	GLN
1	C	62	HIS
1	C	106	ASN
1	C	184	HIS
1	C	596	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	-0.05	8 (1%)	73 46	126, 154, 192, 224	0
1	B	562/675 (83%)	-0.05	6 (1%)	78 52	143, 184, 225, 246	0
1	C	565/675 (83%)	-0.04	8 (1%)	73 46	139, 179, 214, 227	0
All	All	1697/2025 (83%)	-0.05	22 (1%)	75 48	126, 173, 215, 246	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	666	ALA	3.0
1	A	666	ALA	2.9
1	A	663	GLY	2.9
1	C	505	GLY	2.8
1	A	661	THR	2.8
1	B	505	GLY	2.6
1	B	643	THR	2.4
1	A	462	ALA	2.4
1	B	557	TYR	2.3
1	A	505	GLY	2.3
1	B	175	PRO	2.3
1	C	599	GLN	2.3
1	A	112	LEU	2.2
1	C	663	GLY	2.2
1	C	194	CYS	2.2
1	C	628	CYS	2.1
1	B	14	SER	2.1
1	A	571	LEU	2.1
1	C	504	TYR	2.1
1	C	661	THR	2.1
1	A	626	ALA	2.1
1	B	666	ALA	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.