



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:42 am BST

PDB ID : 2UZX
Title : Structure of the human receptor tyrosine kinase Met in complex with the
Listeria monocytogenes invasion protein InlB: Crystal form I
Authors : Niemann, H.H.; Jager, V.; Butler, P.J.G.; Van Den Heuvel, J.; Schmidt, S.;
Ferraris, D.; Gherardi, E.; Heinz, D.W.
Deposited on : 2007-05-02
Resolution : 2.80 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 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 : 2.11
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) : 2.11

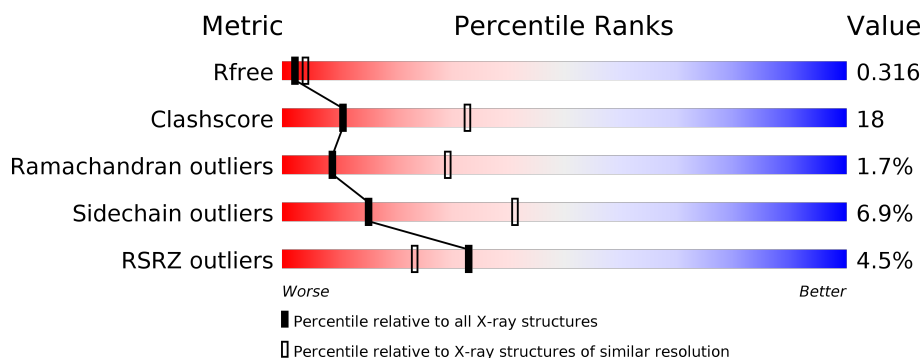
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. 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	289	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
1	C	289	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>..</div> </div> </div>
2	B	727	<div> <div>4%</div> <div> <div></div> <div>45%</div> <div>26%</div> <div>•</div> <div>25%</div> </div> </div>
2	D	727	<div> <div>5%</div> <div> <div></div> <div>45%</div> <div>26%</div> <div>5%</div> <div>25%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13170 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 INTERNALIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2257	1438	379	438	2			
1	C	287	Total	C	N	O	S	0	0	0
			2257	1438	379	438	2			

- Molecule 2 is a protein called HEPATOCYTE GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	547	Total	C	N	O	S	0	0	1
			4328	2757	732	809	30			
2	D	547	Total	C	N	O	S	0	0	1
			4328	2757	732	809	30			

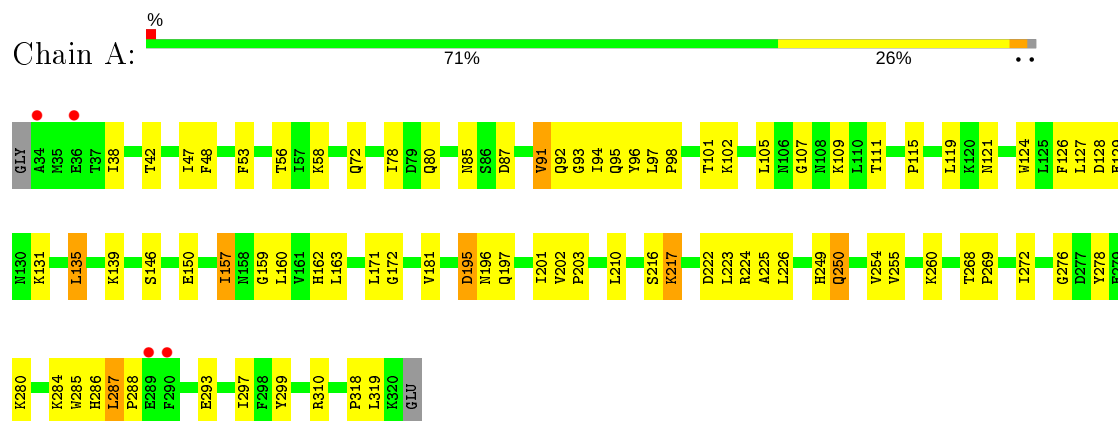
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	CYS	TYR	conflict	UNP P08581
B	344	ALA	GLY	conflict	UNP P08581
D	41	CYS	TYR	conflict	UNP P08581
D	344	ALA	GLY	conflict	UNP P08581

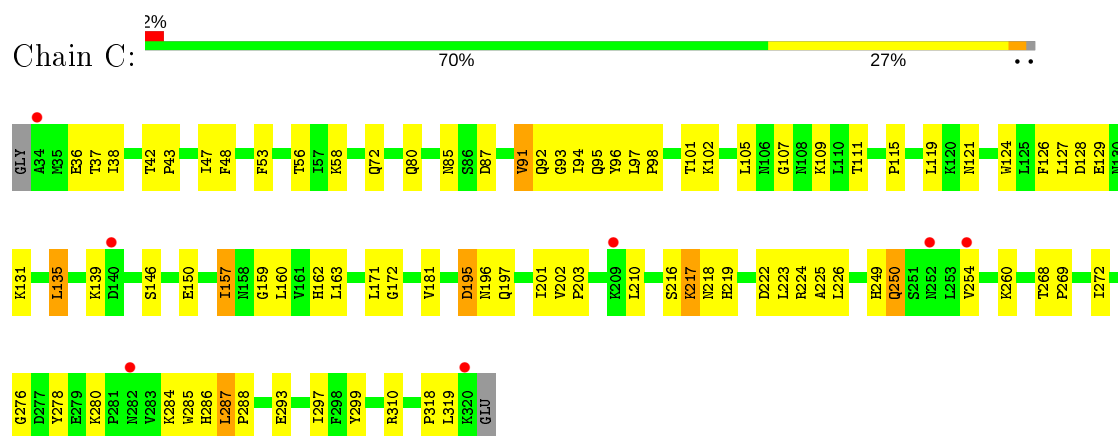
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

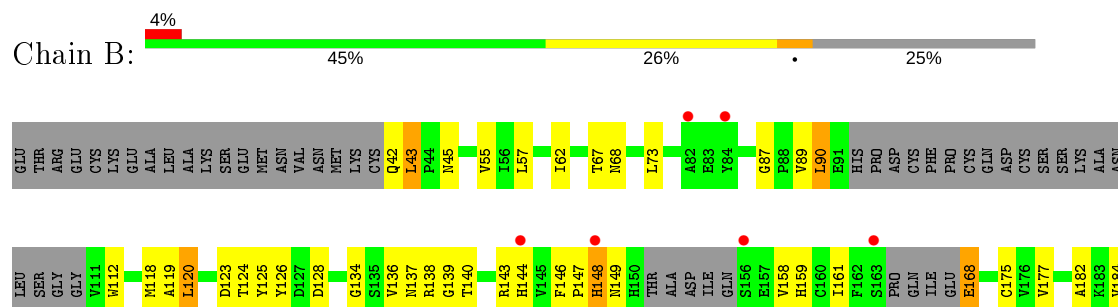
• Molecule 1: INTERNALIN B

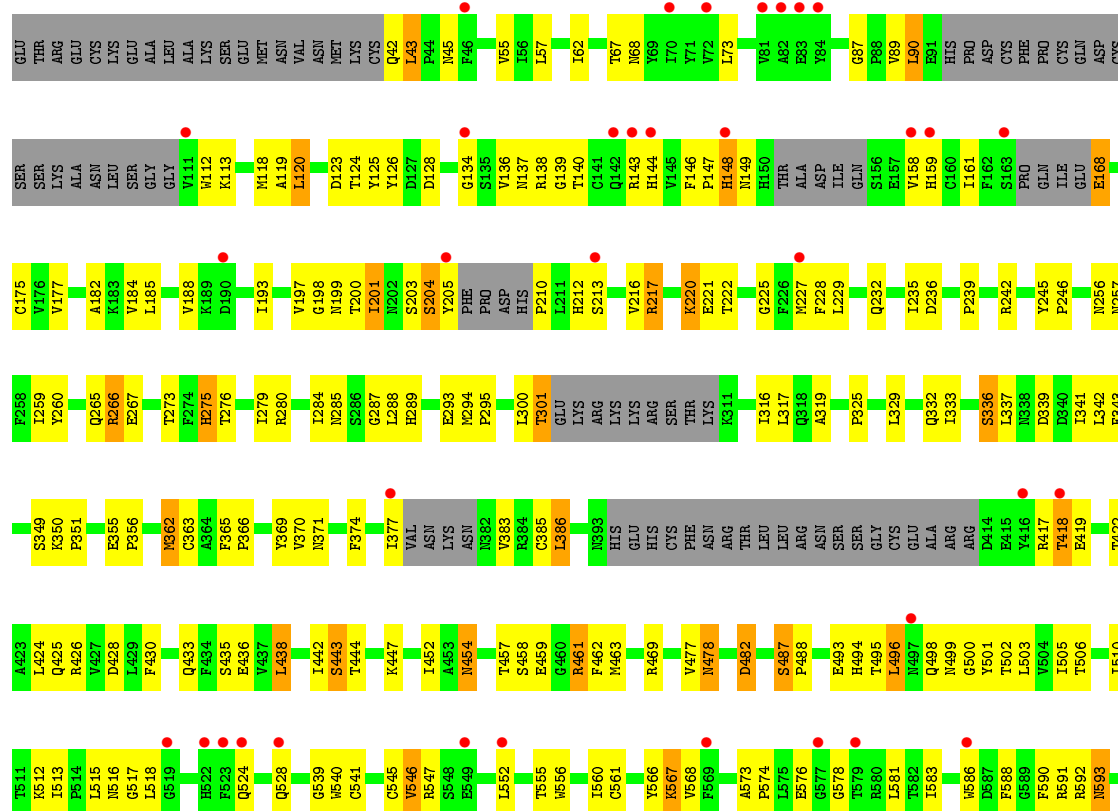


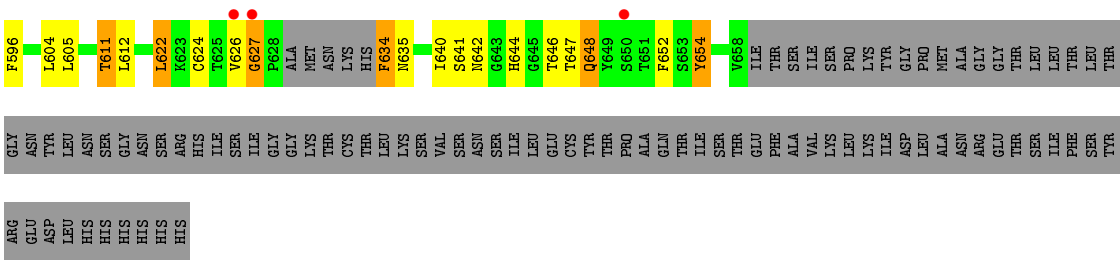
• Molecule 1: INTERNALIN B



• Molecule 2: HEPATOCYTE GROWTH FACTOR RECEPTOR







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.50 Å 66.70 Å 181.50 Å 90.00° 123.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 48.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (15.00-2.80) 97.2 (48.39-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.81 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.268 , 0.307 0.279 , 0.316	Depositor DCC
R_{free} test set	2482 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13170	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.05 % 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 2.8953e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.34	0/2293	0.53	0/3112
1	C	0.34	0/2293	0.53	0/3112
2	B	0.37	0/4427	0.58	0/6001
2	D	0.37	0/4427	0.58	0/6001
All	All	0.36	0/13440	0.56	0/18226

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
2	B	0	3
2	D	0	3
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	168	GLU	Peptide
2	B	210	PRO	Peptide
2	B	627	GLY	Peptide
2	D	168	GLU	Peptide
2	D	210	PRO	Peptide
2	D	627	GLY	Peptide

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	2257	0	2328	69	0
1	C	2257	0	2328	70	0
2	B	4328	0	4212	175	0
2	D	4328	0	4212	171	0
All	All	13170	0	13080	480	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 (480) 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)
2:D:329:LEU:HA	2:D:332:GLN:NE2	1.93	0.84
2:D:43:LEU:HD12	2:D:513:ILE:HA	1.61	0.82
2:B:329:LEU:HA	2:B:332:GLN:NE2	1.93	0.82
2:B:43:LEU:HD12	2:B:513:ILE:HA	1.61	0.80
2:B:647:THR:HG22	2:B:648:GLN:H	1.47	0.80
2:D:647:THR:HG22	2:D:648:GLN:H	1.48	0.79
2:B:546:VAL:HG22	2:B:547:ARG:H	1.48	0.78
1:A:157:ILE:H	1:A:157:ILE:HD13	1.49	0.78
2:D:546:VAL:HG22	2:D:547:ARG:H	1.47	0.78
1:C:157:ILE:H	1:C:157:ILE:HD13	1.49	0.76
2:B:329:LEU:HA	2:B:332:GLN:HE21	1.51	0.76
1:A:80:GLN:HB2	1:A:102:LYS:HB2	1.68	0.76
2:B:161:ILE:HG23	2:B:225:GLY:HA2	1.68	0.75
2:B:265:GLN:O	2:B:275:HIS:HB2	1.87	0.75
1:C:80:GLN:HB2	1:C:102:LYS:HB2	1.68	0.75
2:D:561:CYS:H	2:D:644:HIS:HD2	1.32	0.75
2:D:161:ILE:HG23	2:D:225:GLY:HA2	1.68	0.74
2:D:265:GLN:O	2:D:275:HIS:HB2	1.87	0.74
2:B:611:THR:O	2:B:624:CYS:HB2	1.88	0.73
2:D:611:THR:O	2:D:624:CYS:HB2	1.88	0.73
2:B:89:VAL:HB	2:B:136:VAL:HG11	1.71	0.73
1:A:286:HIS:NE2	1:A:288:PRO:HG3	2.03	0.73
1:A:195:ASP:HA	1:A:217:LYS:HB2	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:LEU:HG	2:B:626:VAL:HG21	1.71	0.72
1:C:195:ASP:HA	1:C:217:LYS:HB2	1.71	0.72
2:D:329:LEU:HA	2:D:332:GLN:HE21	1.50	0.72
1:C:286:HIS:NE2	1:C:288:PRO:HG3	2.04	0.72
2:D:89:VAL:HB	2:D:136:VAL:HG11	1.71	0.72
1:A:85:ASN:O	2:D:496:LEU:HD13	1.90	0.71
1:C:135:LEU:HD13	1:C:159:GLY:HA3	1.72	0.71
2:D:581:LEU:HG	2:D:626:VAL:HG21	1.71	0.71
2:B:300:LEU:HD12	2:B:301:THR:H	1.55	0.71
2:B:566:TYR:O	2:B:567:LYS:HB2	1.90	0.71
1:A:135:LEU:HD13	1:A:159:GLY:HA3	1.72	0.71
2:D:300:LEU:HD12	2:D:301:THR:H	1.55	0.70
2:D:566:TYR:O	2:D:567:LYS:HB2	1.90	0.70
2:B:443:SER:HB2	2:B:454:ASN:OD1	1.90	0.70
2:D:443:SER:HB2	2:D:454:ASN:OD1	1.90	0.70
2:B:583:ILE:HD13	2:B:640:ILE:HD11	1.75	0.68
1:C:87:ASP:OD1	1:C:109:LYS:HE3	1.94	0.68
2:D:216:VAL:CG2	2:D:288:LEU:HD11	2.24	0.67
2:D:583:ILE:HD13	2:D:640:ILE:HD11	1.75	0.67
2:B:216:VAL:CG2	2:B:288:LEU:HD11	2.24	0.67
1:A:87:ASP:OD1	1:A:109:LYS:HE3	1.94	0.66
1:C:286:HIS:CD2	1:C:288:PRO:HG3	2.31	0.66
2:D:498:GLN:HG2	2:D:500:GLY:H	1.61	0.66
1:A:286:HIS:CD2	1:A:288:PRO:HG3	2.31	0.65
2:B:498:GLN:HG2	2:B:500:GLY:H	1.61	0.65
1:C:135:LEU:HD21	1:C:157:ILE:HA	1.79	0.65
2:B:590:PHE:CE1	2:B:644:HIS:CE1	2.85	0.65
2:D:590:PHE:CE1	2:D:644:HIS:CE1	2.85	0.64
1:A:139:LYS:HE2	1:A:162:HIS:CD2	2.32	0.64
2:B:365:PHE:CE2	2:B:426:ARG:HG2	2.33	0.64
2:D:217:ARG:HD2	2:D:217:ARG:H	1.63	0.64
1:A:135:LEU:HD21	1:A:157:ILE:HA	1.79	0.64
1:C:139:LYS:HG2	1:C:162:HIS:CG	2.33	0.64
2:B:43:LEU:HD23	2:B:43:LEU:H	1.63	0.64
1:C:139:LYS:HE2	1:C:162:HIS:CD2	2.32	0.64
2:D:287:GLY:HA2	2:D:289:HIS:NE2	2.14	0.63
2:D:148:HIS:CD2	2:D:149:ASN:H	2.17	0.63
2:D:43:LEU:HD23	2:D:43:LEU:H	1.63	0.63
2:B:217:ARG:HD2	2:B:217:ARG:H	1.63	0.63
2:B:280:ARG:NH2	2:B:374:PHE:HB3	2.14	0.63
1:A:139:LYS:HG2	1:A:162:HIS:CG	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:HA	1:C:107:GLY:O	1.99	0.62
2:D:365:PHE:CE2	2:D:426:ARG:HG2	2.33	0.62
1:A:85:ASN:HA	1:A:107:GLY:O	1.99	0.62
2:B:148:HIS:CD2	2:B:149:ASN:H	2.17	0.62
1:C:226:LEU:H	1:C:226:LEU:HD12	1.65	0.62
2:D:626:VAL:HG12	2:D:654:TYR:OH	2.00	0.62
2:B:626:VAL:HG12	2:B:654:TYR:OH	1.99	0.62
2:D:280:ARG:NH2	2:D:374:PHE:HB3	2.14	0.62
2:B:287:GLY:HA2	2:B:289:HIS:NE2	2.13	0.62
2:D:220:LYS:HD3	2:D:225:GLY:O	2.00	0.61
2:B:220:LYS:HD3	2:B:225:GLY:O	2.00	0.61
2:D:605:LEU:HD21	2:D:652:PHE:CE2	2.36	0.61
2:D:634:PHE:HD1	2:D:635:ASN:H	1.49	0.60
2:B:583:ILE:HG21	2:B:640:ILE:HD11	1.84	0.60
2:D:235:ILE:HD12	2:D:417:ARG:HG2	1.83	0.60
1:A:226:LEU:H	1:A:226:LEU:HD12	1.65	0.60
2:B:634:PHE:HD1	2:B:635:ASN:H	1.49	0.60
2:B:605:LEU:HD21	2:B:652:PHE:CE2	2.36	0.60
1:C:139:LYS:HE2	1:C:162:HIS:NE2	2.16	0.60
1:A:139:LYS:HE2	1:A:162:HIS:NE2	2.16	0.60
1:A:249:HIS:HD2	1:A:287:LEU:HD23	1.67	0.59
2:B:612:LEU:HA	2:B:624:CYS:CB	2.32	0.59
2:D:583:ILE:HG21	2:D:640:ILE:HD11	1.84	0.59
2:B:235:ILE:HD12	2:B:417:ARG:HG2	1.83	0.59
2:B:517:GLY:O	2:B:518:LEU:HD13	2.03	0.59
1:C:249:HIS:HD2	1:C:287:LEU:HD23	1.67	0.58
2:B:430:PHE:HB3	2:B:433:GLN:HB3	1.85	0.58
2:B:216:VAL:HG21	2:B:288:LEU:HD11	1.85	0.58
2:B:611:THR:C	2:B:624:CYS:HB2	2.24	0.58
2:D:517:GLY:O	2:D:518:LEU:HD13	2.03	0.58
2:D:430:PHE:HB3	2:D:433:GLN:HB3	1.84	0.58
2:D:612:LEU:HA	2:D:624:CYS:CB	2.32	0.58
2:D:578:GLY:HA2	2:D:627:GLY:H	1.67	0.58
2:B:578:GLY:HA2	2:B:627:GLY:H	1.67	0.58
2:D:125:TYR:CE1	2:D:188:VAL:HG11	2.38	0.58
2:B:497:ASN:HD22	2:D:555:THR:HA	1.69	0.58
2:D:216:VAL:HG21	2:D:288:LEU:HD11	1.85	0.58
2:D:611:THR:C	2:D:624:CYS:HB2	2.24	0.58
2:B:125:TYR:CE1	2:B:188:VAL:HG11	2.38	0.57
2:B:287:GLY:HA2	2:B:289:HIS:CE1	2.39	0.57
2:D:287:GLY:HA2	2:D:289:HIS:CE1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:HH21	1:A:260:LYS:CD	2.18	0.57
2:B:561:CYS:H	2:B:644:HIS:HD2	1.53	0.57
2:B:216:VAL:HB	2:B:288:LEU:HD11	1.86	0.57
1:A:201:ILE:HG13	1:A:225:ALA:HB3	1.87	0.56
2:B:539:GLY:HA3	2:B:556:TRP:NE1	2.20	0.56
1:C:224:ARG:HH21	1:C:260:LYS:CD	2.18	0.56
2:D:539:GLY:HA3	2:D:556:TRP:NE1	2.19	0.56
2:D:266:ARG:HG2	2:D:266:ARG:O	2.05	0.56
2:B:266:ARG:O	2:B:266:ARG:HG2	2.05	0.56
2:D:216:VAL:HB	2:D:288:LEU:HD11	1.86	0.56
2:D:200:THR:O	2:D:201:ILE:HG23	2.07	0.55
2:D:229:LEU:HD22	2:D:285:ASN:HB3	1.89	0.55
1:C:201:ILE:HG13	1:C:225:ALA:HB3	1.88	0.55
1:A:101:THR:HG22	1:A:121:ASN:O	2.07	0.55
1:A:285:TRP:HB3	1:A:287:LEU:HD13	1.89	0.55
2:B:287:GLY:CA	2:B:289:HIS:NE2	2.69	0.55
1:C:101:THR:HG22	1:C:121:ASN:O	2.07	0.55
2:D:287:GLY:CA	2:D:289:HIS:NE2	2.70	0.54
2:D:583:ILE:HG21	2:D:640:ILE:CD1	2.37	0.54
2:B:592:ARG:HD3	2:B:593:ASN:H	1.73	0.54
2:B:144:HIS:ND1	2:B:158:VAL:HG22	2.22	0.54
2:B:200:THR:O	2:B:201:ILE:HG23	2.07	0.54
1:C:285:TRP:HB3	1:C:287:LEU:HD13	1.89	0.54
2:D:284:ILE:O	2:D:285:ASN:HB2	2.08	0.54
1:A:48:PHE:HA	1:A:92:GLN:O	2.08	0.54
2:B:260:TYR:HA	2:B:279:ILE:O	2.08	0.54
2:B:499:ASN:O	2:B:515:LEU:HB2	2.08	0.54
2:B:647:THR:HG22	2:B:648:GLN:N	2.20	0.54
2:D:118:MET:CB	2:D:177:VAL:HG11	2.38	0.54
2:B:284:ILE:O	2:B:285:ASN:HB2	2.08	0.54
2:B:125:TYR:HE1	1:C:43:PRO:HD3	1.73	0.54
2:B:457:THR:HG22	2:B:458:SER:N	2.22	0.54
2:B:583:ILE:HG21	2:B:640:ILE:CD1	2.37	0.54
2:D:198:GLY:HA2	2:D:213:SER:O	2.08	0.54
2:D:592:ARG:HD3	2:D:593:ASN:H	1.73	0.54
2:D:260:TYR:HA	2:D:279:ILE:O	2.08	0.53
2:D:457:THR:HG22	2:D:458:SER:N	2.22	0.53
2:B:229:LEU:HD22	2:B:285:ASN:HB3	1.89	0.53
1:C:48:PHE:HA	1:C:92:GLN:O	2.08	0.53
2:D:463:MET:HB3	2:D:478:ASN:HA	1.89	0.53
1:C:318:PRO:O	1:C:319:LEU:HD23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:HIS:ND1	2:D:158:VAL:HG22	2.22	0.53
2:B:198:GLY:HA2	2:B:213:SER:O	2.08	0.53
2:B:362:MET:O	2:B:428:ASP:HA	2.08	0.53
2:B:591:ARG:HB2	2:B:596:PHE:CZ	2.43	0.53
2:D:499:ASN:O	2:D:515:LEU:HB2	2.07	0.53
2:B:118:MET:CB	2:B:177:VAL:HG11	2.38	0.53
2:D:316:ILE:O	2:D:316:ILE:HG22	2.09	0.53
1:C:286:HIS:O	1:C:288:PRO:HD3	2.09	0.53
2:D:591:ARG:HB2	2:D:596:PHE:CZ	2.43	0.53
2:D:216:VAL:CB	2:D:288:LEU:HD11	2.39	0.53
2:D:362:MET:O	2:D:428:ASP:HA	2.08	0.53
2:D:424:LEU:HD23	2:D:425:GLN:N	2.24	0.53
2:B:424:LEU:HD23	2:B:425:GLN:N	2.25	0.52
1:A:318:PRO:O	1:A:319:LEU:HD23	2.09	0.52
2:B:463:MET:HB3	2:B:478:ASN:HA	1.90	0.52
2:B:216:VAL:CB	2:B:288:LEU:HD11	2.39	0.52
1:C:285:TRP:HB3	1:C:287:LEU:CD1	2.39	0.52
2:D:647:THR:HG22	2:D:648:GLN:N	2.20	0.52
1:A:285:TRP:HB3	1:A:287:LEU:CD1	2.39	0.52
2:B:482:ASP:OD1	2:B:506:THR:HB	2.09	0.52
2:B:539:GLY:HA3	2:B:556:TRP:CE2	2.44	0.52
2:D:482:ASP:OD1	2:D:506:THR:HB	2.09	0.52
2:D:539:GLY:HA3	2:D:556:TRP:CE2	2.44	0.52
1:A:297:ILE:HD12	1:A:297:ILE:N	2.25	0.52
2:B:452:ILE:HD12	2:B:452:ILE:N	2.25	0.52
2:B:612:LEU:HA	2:B:624:CYS:HB3	1.91	0.52
1:C:128:ASP:OD2	1:C:150:GLU:N	2.32	0.52
2:B:43:LEU:HD11	2:B:513:ILE:HG12	1.92	0.52
1:C:299:TYR:OH	1:C:310:ARG:HD2	2.10	0.52
2:B:498:GLN:HE21	2:B:500:GLY:HA2	1.74	0.52
2:D:452:ILE:N	2:D:452:ILE:HD12	2.25	0.52
2:D:612:LEU:HA	2:D:624:CYS:HB3	1.91	0.52
2:D:612:LEU:HD23	2:D:624:CYS:HB3	1.93	0.51
1:A:128:ASP:OD2	1:A:150:GLU:N	2.32	0.51
2:B:300:LEU:HD12	2:B:301:THR:N	2.25	0.51
2:D:216:VAL:HG23	2:D:288:LEU:HD21	1.92	0.51
2:D:317:LEU:HD11	2:D:319:ALA:O	2.11	0.51
1:C:297:ILE:HD12	1:C:297:ILE:N	2.25	0.51
2:D:540:TRP:CZ3	2:D:545:CYS:HB2	2.45	0.51
1:A:286:HIS:O	1:A:288:PRO:HD3	2.09	0.51
2:B:612:LEU:HD23	2:B:624:CYS:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ILE:HG12	1:C:181:VAL:HG11	1.93	0.51
2:B:342:LEU:HB3	2:B:365:PHE:HB2	1.93	0.51
1:A:97:LEU:O	1:A:119:LEU:HD22	2.11	0.51
2:B:287:GLY:HA3	2:B:289:HIS:CD2	2.45	0.51
2:D:287:GLY:HA3	2:D:289:HIS:CD2	2.45	0.51
2:B:317:LEU:HD11	2:B:319:ALA:O	2.11	0.51
1:A:299:TYR:OH	1:A:310:ARG:HD2	2.10	0.51
2:B:239:PRO:HG3	2:B:242:ARG:NH2	2.26	0.51
2:D:276:THR:HG21	2:D:317:LEU:HB2	1.93	0.51
1:A:139:LYS:HG2	1:A:162:HIS:CD2	2.46	0.50
2:B:288:LEU:HD12	2:B:288:LEU:N	2.26	0.50
2:B:316:ILE:O	2:B:316:ILE:HG22	2.09	0.50
1:C:97:LEU:O	1:C:119:LEU:HD22	2.11	0.50
2:D:288:LEU:N	2:D:288:LEU:HD12	2.27	0.50
2:D:316:ILE:HD13	2:D:349:SER:HB3	1.92	0.50
2:B:143:ARG:HB2	2:B:159:HIS:HB2	1.93	0.50
2:B:216:VAL:HG23	2:B:288:LEU:HD21	1.92	0.50
2:B:454:ASN:HB2	2:B:462:PHE:CZ	2.46	0.50
2:B:563:PRO:HG3	2:B:642:ASN:ND2	2.26	0.50
2:B:316:ILE:HD13	2:B:349:SER:HB3	1.92	0.50
2:D:454:ASN:HB2	2:D:462:PHE:CZ	2.46	0.50
1:A:157:ILE:HG12	1:A:181:VAL:HG11	1.93	0.50
2:D:573:ALA:HB3	2:D:652:PHE:CZ	2.46	0.50
2:B:540:TRP:CZ3	2:B:545:CYS:HB2	2.45	0.50
1:C:124:TRP:CD1	1:C:146:SER:HB3	2.46	0.50
2:D:239:PRO:HG3	2:D:242:ARG:NH2	2.27	0.50
2:D:342:LEU:HB3	2:D:365:PHE:HB2	1.93	0.50
2:D:495:THR:O	2:D:498:GLN:HB3	2.12	0.50
1:A:254:VAL:HG22	1:A:284:LYS:HG2	1.94	0.50
2:B:276:THR:HG21	2:B:317:LEU:HB2	1.93	0.50
1:C:272:ILE:HG21	1:C:276:GLY:HA3	1.93	0.50
1:A:272:ILE:HG21	1:A:276:GLY:HA3	1.94	0.50
2:B:454:ASN:HB2	2:B:462:PHE:CE1	2.47	0.50
1:C:268:THR:HG22	1:C:278:TYR:HE2	1.77	0.50
2:D:447:LYS:HE3	2:D:516:ASN:OD1	2.12	0.50
2:D:498:GLN:HE21	2:D:500:GLY:HA2	1.75	0.50
2:B:495:THR:O	2:B:498:GLN:HB3	2.12	0.49
2:B:573:ALA:HB3	2:B:652:PHE:CZ	2.46	0.49
1:A:224:ARG:NH2	1:A:260:LYS:HD2	2.28	0.49
2:D:43:LEU:HD11	2:D:513:ILE:HG12	1.92	0.49
1:C:139:LYS:HG2	1:C:162:HIS:CD2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:LEU:HD12	2:D:259:ILE:HG23	1.94	0.49
2:B:185:LEU:HD12	2:B:259:ILE:HG23	1.94	0.49
2:B:447:LYS:HE3	2:B:516:ASN:OD1	2.12	0.49
1:C:254:VAL:HG22	1:C:284:LYS:HG2	1.94	0.49
2:D:143:ARG:HB2	2:D:159:HIS:HB2	1.93	0.49
2:D:184:VAL:HG22	2:D:197:VAL:HG22	1.95	0.49
1:C:111:THR:HG22	1:C:131:LYS:HB2	1.94	0.49
1:C:38:ILE:HG12	1:C:72:GLN:OE1	2.13	0.49
2:D:279:ILE:HG13	2:D:293:GLU:HG2	1.95	0.49
1:A:38:ILE:HG12	1:A:72:GLN:OE1	2.13	0.49
2:D:217:ARG:HB3	2:D:228:PHE:CE2	2.48	0.49
1:A:124:TRP:CD1	1:A:146:SER:HB3	2.46	0.49
1:A:202:VAL:N	1:A:203:PRO:CD	2.76	0.49
2:D:560:ILE:HA	2:D:644:HIS:CD2	2.48	0.49
2:D:438:LEU:HB3	2:D:458:SER:HB3	1.95	0.49
2:D:454:ASN:HB2	2:D:462:PHE:CE1	2.47	0.49
2:B:457:THR:HG22	2:B:459:GLU:N	2.27	0.49
2:D:188:VAL:HG22	2:D:193:ILE:HG12	1.95	0.49
2:B:188:VAL:HG22	2:B:193:ILE:HG12	1.95	0.48
2:D:199:ASN:HB2	2:D:212:HIS:O	2.13	0.48
2:B:217:ARG:HB3	2:B:228:PHE:CE2	2.48	0.48
2:B:438:LEU:HB3	2:B:458:SER:HB3	1.94	0.48
2:D:43:LEU:HD12	2:D:512:LYS:O	2.13	0.48
1:A:268:THR:HG22	1:A:278:TYR:HE2	1.77	0.48
2:B:43:LEU:HD12	2:B:512:LYS:O	2.13	0.48
2:D:457:THR:HG22	2:D:459:GLU:N	2.27	0.48
2:B:418:THR:OG1	2:B:419:GLU:N	2.46	0.48
1:C:224:ARG:NH2	1:C:260:LYS:HD2	2.28	0.48
1:C:202:VAL:N	1:C:203:PRO:CD	2.76	0.48
1:A:111:THR:HG22	1:A:131:LYS:HB2	1.95	0.48
2:B:279:ILE:HG13	2:B:293:GLU:HG2	1.95	0.48
2:B:184:VAL:HG22	2:B:197:VAL:HG22	1.95	0.48
2:B:199:ASN:HB2	2:B:212:HIS:O	2.13	0.48
2:B:325:PRO:HG3	2:B:341:ILE:HG13	1.96	0.48
1:C:124:TRP:HB3	1:C:126:PHE:HE1	1.79	0.48
2:D:138:ARG:HH22	2:D:205:TYR:C	2.17	0.47
1:A:201:ILE:HG13	1:A:225:ALA:CB	2.44	0.47
2:B:546:VAL:HG22	2:B:547:ARG:N	2.25	0.47
1:C:58:LYS:C	1:C:58:LYS:HD2	2.35	0.47
2:B:220:LYS:HD2	2:B:227:MET:HG2	1.96	0.47
2:B:493:GLU:HB2	2:B:501:TYR:CZ	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:LYS:HD2	2:D:227:MET:HG2	1.96	0.47
1:A:157:ILE:HB	1:A:160:LEU:HD12	1.97	0.47
2:D:300:LEU:HD12	2:D:301:THR:N	2.25	0.47
2:D:493:GLU:HB2	2:D:501:TYR:CZ	2.49	0.47
2:D:546:VAL:HG22	2:D:547:ARG:N	2.25	0.47
1:A:157:ILE:H	1:A:157:ILE:CD1	2.25	0.47
2:B:232:GLN:HB3	2:B:417:ARG:HH22	1.80	0.47
1:C:111:THR:HG22	1:C:131:LYS:CB	2.44	0.47
1:C:157:ILE:HB	1:C:160:LEU:HD12	1.97	0.47
2:D:325:PRO:HG3	2:D:341:ILE:HG13	1.96	0.47
2:B:581:LEU:HG	2:B:626:VAL:CG2	2.44	0.47
2:D:350:LYS:HB3	2:D:351:PRO:HD2	1.96	0.47
1:A:124:TRP:HB3	1:A:126:PHE:HE1	1.79	0.47
1:A:111:THR:HG22	1:A:131:LYS:CB	2.44	0.47
2:B:137:ASN:HB2	2:B:140:THR:HG22	1.97	0.47
2:B:385:CYS:O	2:B:386:LEU:C	2.53	0.47
2:B:498:GLN:HG2	2:B:499:ASN:N	2.30	0.47
2:D:113:LYS:HE3	2:D:113:LYS:HB3	1.53	0.47
1:C:150:GLU:HG2	1:C:172:GLY:N	2.30	0.47
2:B:217:ARG:HG3	2:B:217:ARG:HH11	1.80	0.46
2:B:148:HIS:CD2	2:B:149:ASN:N	2.83	0.46
1:C:171:LEU:HA	1:C:171:LEU:HD23	1.78	0.46
2:D:498:GLN:HG2	2:D:499:ASN:N	2.30	0.46
1:A:58:LYS:C	1:A:58:LYS:HD2	2.35	0.46
2:B:161:ILE:N	2:B:161:ILE:HD12	2.30	0.46
2:B:540:TRP:HZ3	2:B:545:CYS:HB2	1.81	0.46
2:D:213:SER:OG	2:D:236:ASP:HA	2.15	0.46
2:D:62:ILE:HB	2:D:73:LEU:HB2	1.97	0.46
2:B:138:ARG:HH22	2:B:205:TYR:C	2.17	0.46
1:C:38:ILE:HD11	1:C:72:GLN:N	2.31	0.46
2:D:461:ARG:HE	2:D:461:ARG:HB3	1.59	0.46
2:B:568:VAL:CG1	2:B:581:LEU:HD22	2.45	0.46
2:D:147:PRO:O	2:D:148:HIS:CB	2.63	0.46
2:D:239:PRO:HA	2:D:242:ARG:NE	2.30	0.46
2:D:245:TYR:HA	2:D:246:PRO:HD3	1.61	0.46
2:B:147:PRO:O	2:B:148:HIS:CB	2.63	0.46
1:C:201:ILE:HG13	1:C:225:ALA:CB	2.45	0.46
2:D:137:ASN:HB2	2:D:140:THR:HG22	1.97	0.46
2:D:232:GLN:HB3	2:D:417:ARG:HH22	1.80	0.46
2:D:43:LEU:CD1	2:D:513:ILE:HA	2.40	0.46
1:A:38:ILE:HD11	1:A:72:GLN:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:LYS:HB2	2:B:222:THR:HG22	1.98	0.46
2:B:239:PRO:HA	2:B:242:ARG:NE	2.30	0.46
2:D:568:VAL:CG1	2:D:581:LEU:HD22	2.45	0.46
2:D:641:SER:HB2	2:D:646:THR:HG22	1.98	0.46
1:A:150:GLU:HG2	1:A:172:GLY:N	2.30	0.46
2:B:213:SER:OG	2:B:236:ASP:HA	2.15	0.46
2:D:463:MET:HB2	2:D:477:VAL:O	2.16	0.46
2:D:581:LEU:HG	2:D:626:VAL:CG2	2.44	0.46
2:B:350:LYS:HB3	2:B:351:PRO:HD2	1.96	0.45
2:D:217:ARG:O	2:D:217:ARG:HG2	2.16	0.45
1:A:249:HIS:CD2	1:A:287:LEU:HD23	2.50	0.45
2:D:161:ILE:N	2:D:161:ILE:HD12	2.31	0.45
2:B:377:ILE:HD12	2:B:377:ILE:O	2.17	0.45
2:B:417:ARG:HD2	2:B:417:ARG:N	2.32	0.45
2:B:641:SER:HB2	2:B:646:THR:HG22	1.98	0.45
2:B:642:ASN:OD1	2:B:644:HIS:HB2	2.16	0.45
2:B:62:ILE:HB	2:B:73:LEU:HB2	1.97	0.45
2:D:385:CYS:O	2:D:386:LEU:C	2.53	0.45
2:B:457:THR:HG22	2:B:459:GLU:H	1.82	0.45
2:B:329:LEU:CD1	2:B:333:ILE:HD13	2.47	0.45
1:A:96:TYR:O	1:A:98:PRO:HD3	2.17	0.45
2:B:256:ASN:O	2:B:257:ASN:HB2	2.17	0.45
2:B:370:VAL:HG12	2:B:371:ASN:N	2.32	0.45
2:B:590:PHE:CE1	2:B:644:HIS:ND1	2.85	0.45
2:D:418:THR:OG1	2:D:419:GLU:N	2.47	0.45
2:D:457:THR:CG2	2:D:458:SER:N	2.80	0.45
2:D:503:LEU:HB3	2:D:510:ILE:HD11	1.99	0.45
2:D:540:TRP:HZ3	2:D:545:CYS:HB2	1.81	0.45
2:D:590:PHE:CE1	2:D:644:HIS:ND1	2.85	0.45
2:D:561:CYS:H	2:D:644:HIS:CD2	2.22	0.45
2:B:43:LEU:CD1	2:B:513:ILE:HA	2.40	0.45
2:B:605:LEU:HD22	2:B:626:VAL:HG13	1.99	0.45
1:C:272:ILE:CG2	1:C:276:GLY:HA3	2.47	0.45
2:D:220:LYS:HB2	2:D:222:THR:HG22	1.98	0.45
2:D:256:ASN:O	2:D:257:ASN:HB2	2.17	0.45
2:D:417:ARG:N	2:D:417:ARG:HD2	2.31	0.45
2:B:457:THR:CG2	2:B:458:SER:N	2.80	0.45
2:B:463:MET:HB2	2:B:477:VAL:O	2.17	0.45
2:D:329:LEU:CD1	2:D:333:ILE:HD13	2.47	0.45
1:A:272:ILE:CG2	1:A:276:GLY:HA3	2.47	0.44
1:A:128:ASP:O	1:A:129:GLU:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:HIS:CD2	2:D:149:ASN:N	2.83	0.44
2:D:642:ASN:OD1	2:D:644:HIS:HB2	2.16	0.44
2:B:182:ALA:HA	2:B:198:GLY:O	2.17	0.44
2:B:161:ILE:CG2	2:B:225:GLY:HA2	2.44	0.44
2:B:496:LEU:HD13	1:C:85:ASN:O	2.17	0.44
2:B:503:LEU:HB3	2:B:510:ILE:HD11	1.99	0.44
2:B:217:ARG:O	2:B:217:ARG:HG2	2.16	0.44
1:C:201:ILE:CD1	1:C:226:LEU:HD11	2.47	0.44
2:D:217:ARG:HG3	2:D:217:ARG:HH11	1.81	0.44
1:A:201:ILE:CD1	1:A:226:LEU:HD11	2.47	0.44
1:C:96:TYR:O	1:C:98:PRO:HD3	2.17	0.44
2:D:605:LEU:HD22	2:D:626:VAL:HG13	1.99	0.44
2:B:284:ILE:HD13	2:B:289:HIS:HD2	1.83	0.44
2:D:137:ASN:HB2	2:D:140:THR:CG2	2.48	0.44
2:D:67:THR:O	2:D:68:ASN:HB2	2.18	0.44
2:D:366:PRO:O	2:D:369:TYR:HB3	2.17	0.44
2:D:457:THR:HG22	2:D:459:GLU:H	1.81	0.44
2:D:329:LEU:HD13	2:D:333:ILE:HD13	2.00	0.44
2:B:90:LEU:HD23	2:B:90:LEU:H	1.83	0.43
1:C:105:LEU:HB2	1:C:127:LEU:HD23	2.00	0.43
1:C:157:ILE:H	1:C:157:ILE:CD1	2.25	0.43
2:D:377:ILE:HD12	2:D:377:ILE:O	2.17	0.43
2:B:461:ARG:HE	2:B:461:ARG:HB3	1.60	0.43
2:B:67:THR:O	2:B:68:ASN:HB2	2.18	0.43
1:C:249:HIS:CD2	1:C:287:LEU:HD23	2.50	0.43
2:D:284:ILE:HD13	2:D:289:HIS:HD2	1.83	0.43
1:A:269:PRO:HD2	1:A:278:TYR:CD2	2.54	0.43
2:B:55:VAL:CG2	2:B:505:ILE:HD11	2.49	0.43
2:B:566:TYR:HB2	2:B:586:TRP:CZ3	2.53	0.43
1:C:42:THR:HB	1:C:47:ILE:HD11	2.00	0.43
2:D:370:VAL:HG12	2:D:371:ASN:N	2.32	0.43
2:D:566:TYR:HB2	2:D:586:TRP:CZ3	2.53	0.43
2:B:329:LEU:HD13	2:B:333:ILE:HD13	2.00	0.43
2:B:366:PRO:O	2:B:369:TYR:HB3	2.17	0.43
1:C:250:GLN:HE21	1:C:250:GLN:HB2	1.67	0.43
2:D:146:PHE:HA	2:D:147:PRO:HD3	1.79	0.43
1:A:196:ASN:HB3	1:A:197:GLN:H	1.58	0.43
2:B:284:ILE:H	2:B:287:GLY:H	1.66	0.43
2:D:182:ALA:HA	2:D:198:GLY:O	2.17	0.43
2:B:245:TYR:HA	2:B:246:PRO:HD3	1.61	0.43
1:C:269:PRO:HD2	1:C:278:TYR:CD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:GLY:HA3	2:D:515:LEU:HD12	2.01	0.43
1:A:105:LEU:HB2	1:A:127:LEU:HD23	2.00	0.43
2:B:43:LEU:H	2:B:43:LEU:CD2	2.31	0.43
1:A:95:GLN:CD	1:A:95:GLN:H	2.22	0.43
1:C:128:ASP:O	1:C:129:GLU:HB2	2.17	0.43
2:D:138:ARG:NH1	2:D:205:TYR:O	2.52	0.43
2:D:55:VAL:CG2	2:D:505:ILE:HD11	2.48	0.43
2:B:588:PHE:CD2	2:B:622:LEU:HD13	2.54	0.43
2:B:566:TYR:CG	2:B:566:TYR:O	2.72	0.42
2:D:138:ARG:HG3	2:D:175:CYS:HB3	2.01	0.42
2:D:343:PHE:CE1	2:D:444:THR:HG21	2.54	0.42
2:B:137:ASN:HB2	2:B:140:THR:CG2	2.48	0.42
1:C:223:LEU:HB3	1:C:226:LEU:HD13	2.00	0.42
2:B:125:TYR:CE1	1:C:43:PRO:HD3	2.54	0.42
1:C:157:ILE:HB	1:C:160:LEU:CD1	2.49	0.42
1:C:95:GLN:H	1:C:95:GLN:CD	2.22	0.42
1:A:223:LEU:HB3	1:A:226:LEU:HD13	2.00	0.42
1:A:42:THR:HB	1:A:47:ILE:HD11	2.00	0.42
2:D:494:HIS:HB2	2:D:515:LEU:CD1	2.49	0.42
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.84	0.42
2:B:138:ARG:NH1	2:B:205:TYR:O	2.52	0.42
2:B:500:GLY:HA3	2:B:515:LEU:HD12	2.01	0.42
2:B:567:LYS:HD2	2:B:567:LYS:HA	1.88	0.42
2:D:90:LEU:H	2:D:90:LEU:HD23	1.84	0.42
1:A:94:ILE:HG22	1:A:115:PRO:HB3	2.01	0.42
2:B:343:PHE:CE1	2:B:444:THR:HG21	2.54	0.42
2:D:119:ALA:O	2:D:120:LEU:HD13	2.20	0.42
2:D:294:MET:HA	2:D:295:PRO:HD3	1.74	0.42
2:D:566:TYR:CG	2:D:566:TYR:O	2.72	0.42
1:A:157:ILE:N	1:A:157:ILE:HD13	2.26	0.42
2:D:284:ILE:HB	2:D:289:HIS:CD2	2.55	0.42
1:A:53:PHE:O	1:A:56:THR:HB	2.19	0.42
2:B:484:HIS:HA	2:B:485:PRO:HD3	1.94	0.42
1:C:196:ASN:HB3	1:C:197:GLN:H	1.57	0.42
1:C:53:PHE:O	1:C:56:THR:HB	2.19	0.42
1:A:157:ILE:HB	1:A:160:LEU:CD1	2.49	0.42
2:B:119:ALA:O	2:B:120:LEU:HD13	2.20	0.42
2:B:355:GLU:HA	2:B:356:PRO:HD3	1.85	0.42
1:C:94:ILE:HG22	1:C:115:PRO:HB3	2.02	0.42
2:D:355:GLU:HA	2:D:356:PRO:HD3	1.85	0.42
1:A:48:PHE:CE1	1:A:93:GLY:O	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:HIS:HB2	2:B:515:LEU:CD1	2.49	0.41
2:D:43:LEU:CD2	2:D:43:LEU:H	2.31	0.41
2:B:138:ARG:HG3	2:B:175:CYS:HB3	2.01	0.41
2:B:267:GLU:HA	2:B:275:HIS:ND1	2.35	0.41
2:B:350:LYS:HB3	2:B:351:PRO:CD	2.50	0.41
2:D:284:ILE:H	2:D:287:GLY:H	1.67	0.41
2:B:325:PRO:HD3	2:B:339:ASP:O	2.20	0.41
1:C:216:SER:C	1:C:217:LYS:HG2	2.41	0.41
1:C:218:ASN:HB3	1:C:219:HIS:H	1.71	0.41
2:D:524:GLN:HB2	2:D:528:GLN:HE22	1.86	0.41
2:B:627:GLY:HA2	2:B:654:TYR:OH	2.21	0.41
2:D:588:PHE:CD2	2:D:622:LEU:HD13	2.54	0.41
1:A:171:LEU:HA	1:A:171:LEU:HD23	1.78	0.41
1:A:268:THR:HA	1:A:269:PRO:HD3	1.86	0.41
2:D:134:GLY:O	2:D:139:GLY:HA2	2.20	0.41
2:D:203:SER:O	2:D:204:SER:HB3	2.20	0.41
1:C:268:THR:HA	1:C:269:PRO:HD3	1.86	0.41
2:D:284:ILE:H	2:D:287:GLY:HA3	1.86	0.41
1:A:216:SER:C	1:A:217:LYS:HG2	2.41	0.41
2:B:124:THR:HG22	2:B:128:ASP:HA	2.03	0.41
2:B:336:SER:O	2:B:339:ASP:HB2	2.21	0.41
2:D:336:SER:O	2:D:339:ASP:HB2	2.21	0.41
2:D:647:THR:CG2	2:D:648:GLN:H	2.26	0.41
2:B:284:ILE:HB	2:B:289:HIS:CD2	2.55	0.41
2:B:612:LEU:HA	2:B:624:CYS:HB2	2.03	0.41
2:D:487:SER:HA	2:D:488:PRO:HD3	1.85	0.41
2:D:573:ALA:HA	2:D:574:PRO:HD3	1.82	0.41
2:B:134:GLY:O	2:B:139:GLY:HA2	2.21	0.41
2:B:647:THR:CG2	2:B:648:GLN:H	2.26	0.41
1:C:48:PHE:CE1	1:C:93:GLY:O	2.73	0.41
1:A:224:ARG:NH2	1:A:260:LYS:CD	2.84	0.41
2:B:146:PHE:HA	2:B:147:PRO:HD3	1.79	0.41
2:B:229:LEU:CD2	2:B:285:ASN:HB3	2.51	0.41
2:D:612:LEU:HA	2:D:624:CYS:HB2	2.03	0.41
2:D:124:THR:HG22	2:D:128:ASP:HA	2.03	0.40
2:D:267:GLU:HA	2:D:275:HIS:ND1	2.35	0.40
1:A:250:GLN:HB2	1:A:250:GLN:HE21	1.68	0.40
1:A:255:VAL:HB	1:A:285:TRP:HZ3	1.86	0.40
2:D:325:PRO:HD3	2:D:339:ASP:O	2.21	0.40
2:B:515:LEU:HD23	2:B:515:LEU:HA	1.84	0.40
2:B:524:GLN:HB2	2:B:528:GLN:HE22	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:LEU:HD12	2:B:605:LEU:HA	1.93	0.40
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.84	0.40
1:C:226:LEU:HD12	1:C:226:LEU:N	2.34	0.40
1:C:36:GLU:O	1:C:37:THR:HB	2.22	0.40
1:A:78:ILE:HD12	1:A:97:LEU:HD21	2.04	0.40
2:B:604:LEU:HD12	2:B:606:GLY:O	2.22	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	285/289 (99%)	253 (89%)	30 (10%)	2 (1%)	22	53
1	C	285/289 (99%)	252 (88%)	31 (11%)	2 (1%)	22	53
2	B	529/727 (73%)	450 (85%)	67 (13%)	12 (2%)	6	21
2	D	529/727 (73%)	451 (85%)	66 (12%)	12 (2%)	6	21
All	All	1628/2032 (80%)	1406 (86%)	194 (12%)	28 (2%)	9	29

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	148	HIS
2	D	148	HIS
2	B	87	GLY
2	B	386	LEU
2	B	552	LEU
2	D	87	GLY
2	D	386	LEU
2	D	552	LEU
2	B	204	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	478	ASN
2	B	546	VAL
2	B	567	LYS
2	D	204	SER
2	D	478	ASN
2	D	546	VAL
2	D	567	LYS
2	B	266	ARG
2	B	482	ASP
2	B	593	ASN
2	D	266	ARG
2	D	482	ASP
2	D	593	ASN
1	A	280	LYS
1	C	280	LYS
2	B	126	TYR
2	D	126	TYR
1	A	91	VAL
1	C	91	VAL

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	264/265 (100%)	254 (96%)	10 (4%)	33	67
1	C	264/265 (100%)	254 (96%)	10 (4%)	33	67
2	B	493/654 (75%)	451 (92%)	42 (8%)	10	31
2	D	493/654 (75%)	451 (92%)	42 (8%)	10	31
All	All	1514/1838 (82%)	1410 (93%)	104 (7%)	15	41

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	VAL
1	A	135	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	157	ILE
1	A	163	LEU
1	A	195	ASP
1	A	217	LYS
1	A	222	ASP
1	A	250	GLN
1	A	287	LEU
1	A	293	GLU
2	B	42	GLN
2	B	43	LEU
2	B	45	ASN
2	B	57	LEU
2	B	90	LEU
2	B	112	TRP
2	B	120	LEU
2	B	123	ASP
2	B	168	GLU
2	B	201	ILE
2	B	217	ARG
2	B	220	LYS
2	B	221	GLU
2	B	273	THR
2	B	275	HIS
2	B	301	THR
2	B	336	SER
2	B	337	LEU
2	B	362	MET
2	B	363	CYS
2	B	383	VAL
2	B	418	THR
2	B	422	THR
2	B	435	SER
2	B	436	GLU
2	B	438	LEU
2	B	442	ILE
2	B	443	SER
2	B	454	ASN
2	B	461	ARG
2	B	469	ARG
2	B	487	SER
2	B	496	LEU
2	B	502	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	541	CYS
2	B	576	GLU
2	B	604	LEU
2	B	611	THR
2	B	622	LEU
2	B	634	PHE
2	B	648	GLN
2	B	654	TYR
1	C	91	VAL
1	C	135	LEU
1	C	157	ILE
1	C	163	LEU
1	C	195	ASP
1	C	217	LYS
1	C	222	ASP
1	C	250	GLN
1	C	287	LEU
1	C	293	GLU
2	D	42	GLN
2	D	43	LEU
2	D	45	ASN
2	D	57	LEU
2	D	90	LEU
2	D	112	TRP
2	D	120	LEU
2	D	123	ASP
2	D	168	GLU
2	D	201	ILE
2	D	217	ARG
2	D	220	LYS
2	D	221	GLU
2	D	273	THR
2	D	275	HIS
2	D	301	THR
2	D	336	SER
2	D	337	LEU
2	D	362	MET
2	D	363	CYS
2	D	383	VAL
2	D	418	THR
2	D	422	THR
2	D	435	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	436	GLU
2	D	438	LEU
2	D	442	ILE
2	D	443	SER
2	D	454	ASN
2	D	461	ARG
2	D	469	ARG
2	D	487	SER
2	D	496	LEU
2	D	502	THR
2	D	541	CYS
2	D	576	GLU
2	D	604	LEU
2	D	611	THR
2	D	622	LEU
2	D	634	PHE
2	D	648	GLN
2	D	654	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
2	B	45	ASN
2	B	148	HIS
2	B	265	GLN
2	B	285	ASN
2	B	289	HIS
2	B	332	GLN
2	B	494	HIS
2	B	498	GLN
1	C	250	GLN
2	D	45	ASN
2	D	148	HIS
2	D	265	GLN
2	D	285	ASN
2	D	289	HIS
2	D	332	GLN
2	D	494	HIS
2	D	498	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	287/289 (99%)	-0.01	4 (1%) 75 70	29, 55, 82, 116	0
1	C	287/289 (99%)	0.10	7 (2%) 59 49	36, 60, 91, 111	0
2	B	547/727 (75%)	0.10	26 (4%) 30 21	17, 55, 95, 119	0
2	D	547/727 (75%)	0.46	38 (6%) 16 10	43, 74, 117, 155	0
All	All	1668/2032 (82%)	0.20	75 (4%) 33 23	17, 62, 103, 155	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	82	ALA	7.0
2	D	84	TYR	5.6
1	C	34	ALA	5.1
2	B	576	GLU	5.0
2	D	416	TYR	5.0
2	D	377	ILE	4.8
1	C	254	VAL	4.7
2	D	70	ILE	4.5
2	D	134	GLY	4.5
2	D	586	TRP	4.4
2	B	524	GLN	4.3
2	D	111	VAL	4.3
1	A	34	ALA	4.1
2	D	163	SER	4.1
2	B	522	HIS	4.1
2	D	83	GLU	4.0
2	B	586	TRP	4.0
2	D	148	HIS	3.9
2	D	522	HIS	3.9
2	D	552	LEU	3.9
2	B	577	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	627	GLY	3.8
2	D	523	PHE	3.6
1	C	320	LYS	3.5
2	D	46	PHE	3.3
2	D	519	GLY	3.3
2	B	148	HIS	3.3
2	B	84	TYR	3.2
2	B	416	TYR	3.2
2	D	418	THR	3.2
1	C	140	ASP	3.1
2	B	523	PHE	3.1
2	D	577	GLY	3.1
1	C	282	ASN	3.1
2	B	156	SER	3.0
2	B	377	ILE	3.0
2	D	205	TYR	3.0
2	D	144	HIS	2.9
1	A	36	GLU	2.9
2	D	497	ASN	2.9
2	D	72	VAL	2.8
2	D	142	GLN	2.7
1	C	209	LYS	2.7
2	D	524	GLN	2.7
2	B	82	ALA	2.7
1	C	252	ASN	2.6
2	D	569	PHE	2.6
2	D	143	ARG	2.6
2	B	569	PHE	2.5
2	B	144	HIS	2.5
2	D	159	HIS	2.5
2	B	205	TYR	2.4
2	D	549	GLU	2.4
2	B	627	GLY	2.4
2	D	227	MET	2.4
2	B	204	SER	2.4
2	D	528	GLN	2.4
2	B	575	LEU	2.3
2	B	163	SER	2.3
2	D	213	SER	2.3
2	B	581	LEU	2.3
1	A	289	GLU	2.3
2	B	628	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	571	ASN	2.2
2	D	650	SER	2.2
2	B	654	TYR	2.2
2	D	579	THR	2.2
2	B	497	ASN	2.2
2	D	81	VAL	2.2
2	D	158	VAL	2.1
2	B	528	GLN	2.1
1	A	290	PHE	2.1
2	B	585	GLY	2.1
2	D	626	VAL	2.1
2	D	190	ASP	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 carbohydrates 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.