



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:44 pm BST

PDB ID : 1ELO
Title : ELONGATION FACTOR G WITHOUT NUCLEOTIDE
Authors : Aevarsson, A.; Brazhnikov, E.; Garber, M.; Zheltonosova, J.; Chirgadze, Yu.;
Al-Karadaghi, S.; Svensson, L.A.; Liljas, A.
Deposited on : 1996-03-13
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

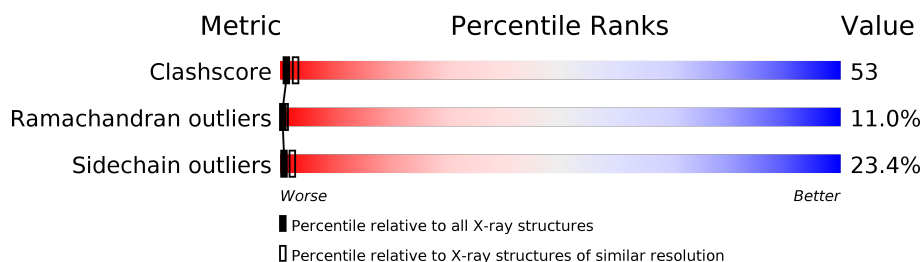
1 Overall quality at a glance

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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	691	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4957 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 ELONGATION FACTOR G.

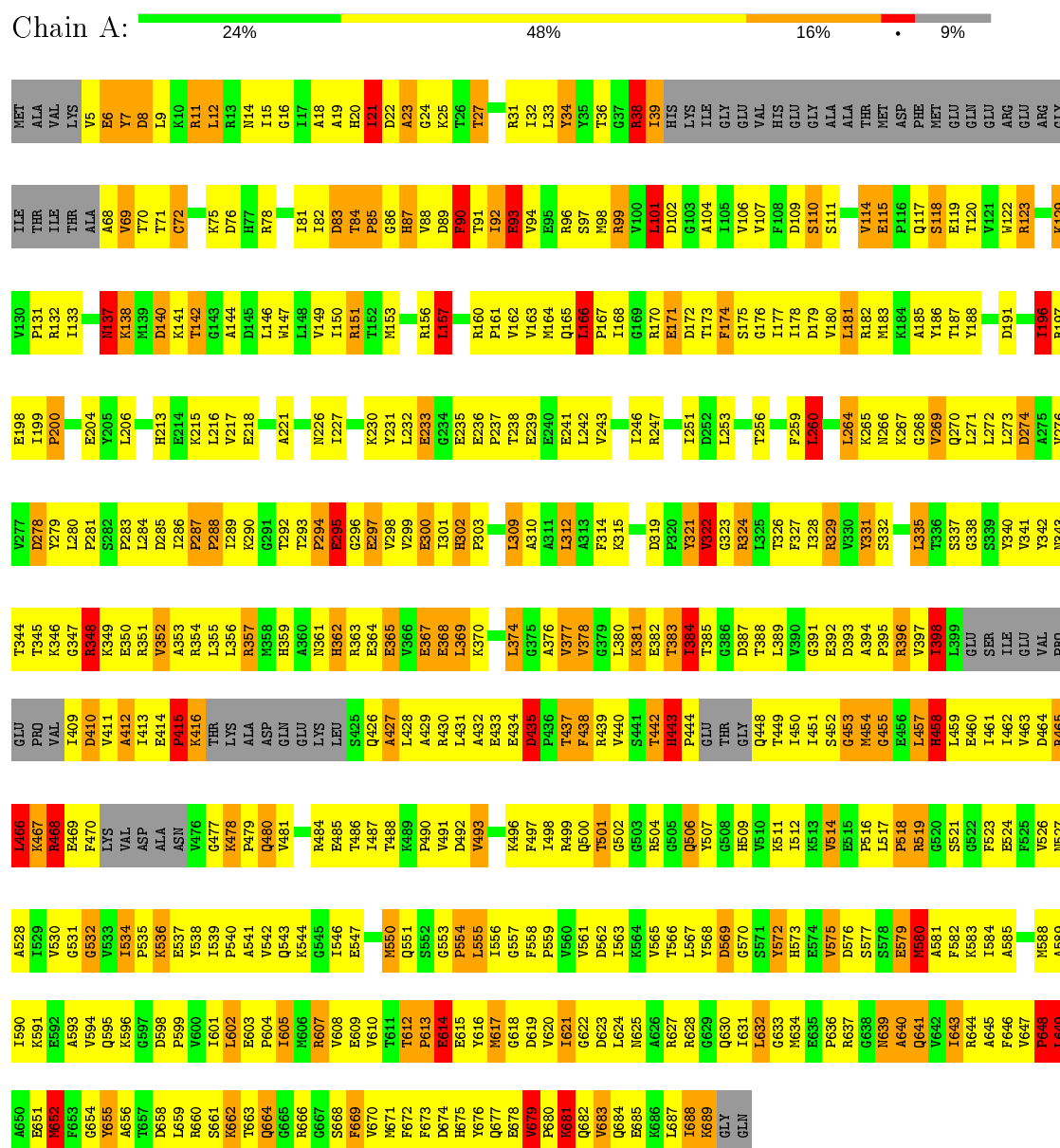
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	632	4957	3157	849	933	18	0	0	0

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: ELONGATION FACTOR G



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.60 Å 106.00 Å 116.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4957	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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	0.91	2/5048 (0.0%)	1.11	25/6829 (0.4%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	PHE	CD1-CE1	5.16	1.49	1.39
1	A	90	PHE	CD2-CE2	5.06	1.49	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	LEU	CA-CB-CG	7.66	132.92	115.30
1	A	534	ILE	N-CA-C	-7.61	90.45	111.00
1	A	466	LEU	CA-CB-CG	7.04	131.49	115.30
1	A	295	GLU	N-CA-C	-6.99	92.13	111.00
1	A	412	ALA	N-CA-C	6.33	128.11	111.00
1	A	351	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	A	649	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	398	ILE	N-CA-C	-5.90	95.06	111.00
1	A	21	ILE	CB-CA-C	-5.82	99.97	111.60
1	A	613	PRO	N-CA-C	-5.81	97.00	112.10
1	A	216	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	443	HIS	N-CA-C	5.59	126.09	111.00
1	A	312	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	679	VAL	N-CA-C	-5.52	96.09	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	VAL	N-CA-C	5.50	125.85	111.00
1	A	458	HIS	N-CA-C	-5.43	96.33	111.00
1	A	466	LEU	N-CA-C	-5.41	96.39	111.00
1	A	8	ASP	N-CA-C	-5.41	96.40	111.00
1	A	260	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	349	LYS	N-CA-C	-5.34	96.57	111.00
1	A	101	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	453	GLY	N-CA-C	5.30	126.36	113.10
1	A	200	PRO	N-CA-C	-5.27	98.40	112.10
1	A	465	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	157	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	TYR	Sidechain

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	4957	0	5021	528	0
All	All	4957	0	5021	528	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 53.

All (528) 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:A:580:MET:CE	1:A:580:MET:SD	2.01	1.48
1:A:346:LYS:HD3	1:A:384:ILE:HD11	1.46	0.97
1:A:289:ILE:HG23	1:A:301:ILE:HB	1.45	0.97
1:A:457:LEU:HG	1:A:460:GLU:HB2	1.45	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HG2	1:A:7:TYR:H	1.32	0.94
1:A:528:ALA:HB3	1:A:568:TYR:HA	1.51	0.93
1:A:9:LEU:HD21	1:A:303:PRO:HB2	1.49	0.92
1:A:335:LEU:HD21	1:A:355:LEU:HD21	1.51	0.91
1:A:213:HIS:O	1:A:217:VAL:HG23	1.73	0.87
1:A:92:ILE:HD11	1:A:454:MET:SD	2.14	0.87
1:A:87:HIS:NE2	1:A:90:PHE:HB2	1.90	0.86
1:A:85:PRO:HG3	1:A:94:VAL:HA	1.58	0.86
1:A:156:ARG:HD2	1:A:666:ARG:HH12	1.39	0.85
1:A:535:PRO:HD3	1:A:572:TYR:CD2	2.13	0.84
1:A:99:ARG:HD3	1:A:99:ARG:O	1.77	0.84
1:A:493:VAL:HG21	1:A:593:ALA:HB2	1.60	0.84
1:A:444:PRO:HA	1:A:448:GLN:HG3	1.59	0.83
1:A:628:ARG:HD2	1:A:648:PRO:HG2	1.61	0.82
1:A:511:LYS:HD2	1:A:569:ASP:HB3	1.61	0.81
1:A:290:LYS:HB3	1:A:298:VAL:HG12	1.62	0.81
1:A:357:ARG:HH11	1:A:357:ARG:HG3	1.44	0.80
1:A:411:VAL:HB	1:A:453:GLY:HA3	1.61	0.80
1:A:27:THR:O	1:A:31:ARG:HG2	1.82	0.80
1:A:411:VAL:HB	1:A:453:GLY:CA	2.12	0.79
1:A:439:ARG:HB2	1:A:439:ARG:HH11	1.47	0.79
1:A:499:ARG:HH11	1:A:499:ARG:HG3	1.46	0.78
1:A:359:HIS:HB2	1:A:362:HIS:O	1.83	0.77
1:A:671:MET:C	1:A:672:PHE:HD1	1.87	0.77
1:A:346:LYS:NZ	1:A:383:THR:HA	1.99	0.77
1:A:247:ARG:HG3	1:A:279:TYR:HA	1.65	0.77
1:A:156:ARG:HD2	1:A:666:ARG:NH1	2.00	0.76
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.51	0.76
1:A:478:LYS:O	1:A:480:GLN:HG3	1.87	0.75
1:A:120:THR:HA	1:A:123:ARG:HG3	1.69	0.75
1:A:624:LEU:HD23	1:A:631:ILE:HD11	1.67	0.75
1:A:647:VAL:HG11	1:A:652:MET:SD	2.27	0.74
1:A:610:VAL:HG13	1:A:659:LEU:HD21	1.68	0.74
1:A:296:GLY:O	1:A:297:GLU:HB2	1.86	0.74
1:A:434:GLU:O	1:A:435:ASP:HB2	1.87	0.74
1:A:481:VAL:HG13	1:A:649:LEU:HD12	1.70	0.74
1:A:630:GLN:HB2	1:A:646:PHE:HB2	1.68	0.74
1:A:346:LYS:HZ2	1:A:383:THR:HA	1.53	0.74
1:A:176:GLY:HA2	1:A:187:THR:HA	1.70	0.73
1:A:276:VAL:HG13	1:A:280:LEU:HD12	1.69	0.73
1:A:658:ASP:O	1:A:662:LYS:HG2	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:HG3	1:A:160:ARG:HH11	1.53	0.73
1:A:309:LEU:HG	1:A:310:ALA:N	2.03	0.73
1:A:129:LYS:O	1:A:131:PRO:HD3	1.89	0.73
1:A:539:ILE:HB	1:A:540:PRO:HD3	1.69	0.73
1:A:484:ARG:HB2	1:A:602:LEU:HB2	1.71	0.73
1:A:468:ARG:NE	1:A:468:ARG:HA	2.05	0.72
1:A:170:ARG:H	1:A:173:THR:HB	1.54	0.72
1:A:535:PRO:HD3	1:A:572:TYR:HD2	1.52	0.72
1:A:6:GLU:HG2	1:A:7:TYR:N	2.04	0.72
1:A:577:SER:HB3	1:A:582:PHE:HE1	1.54	0.72
1:A:413:ILE:HD11	1:A:454:MET:O	1.89	0.71
1:A:181:LEU:HD12	1:A:181:LEU:O	1.90	0.71
1:A:514:VAL:HG21	1:A:593:ALA:HB1	1.71	0.71
1:A:621:ILE:HD11	1:A:643:ILE:HG21	1.71	0.71
1:A:673:PHE:CZ	1:A:675:HIS:HA	2.26	0.71
1:A:85:PRO:CG	1:A:94:VAL:HA	2.20	0.71
1:A:426:GLN:HE21	1:A:430:ARG:NH2	1.88	0.71
1:A:519:ARG:HB2	1:A:519:ARG:HH11	1.54	0.71
1:A:613:PRO:HA	1:A:640:ALA:CB	2.21	0.71
1:A:68:ALA:O	1:A:69:VAL:HG23	1.91	0.71
1:A:348:ARG:NH2	1:A:381:LYS:HE3	2.05	0.71
1:A:164:MET:HE1	1:A:246:ILE:HG21	1.73	0.71
1:A:344:THR:OG1	1:A:388:THR:HB	1.91	0.70
1:A:290:LYS:HA	1:A:299:VAL:O	1.91	0.70
1:A:346:LYS:HE3	1:A:382:GLU:O	1.92	0.70
1:A:185:ALA:HB3	1:A:199:ILE:HG13	1.74	0.70
1:A:591:LYS:O	1:A:595:GLN:HG2	1.92	0.70
1:A:439:ARG:CB	1:A:439:ARG:HH11	2.05	0.69
1:A:680:PRO:O	1:A:683:VAL:HG23	1.92	0.69
1:A:274:ASP:O	1:A:278:ASP:HB2	1.91	0.69
1:A:5:VAL:HG22	1:A:6:GLU:N	2.08	0.69
1:A:617:MET:O	1:A:617:MET:SD	2.50	0.69
1:A:636:PRO:HA	1:A:641:GLN:HG2	1.75	0.69
1:A:612:THR:O	1:A:640:ALA:HB1	1.92	0.69
1:A:92:ILE:O	1:A:93:GLU:HB2	1.91	0.69
1:A:613:PRO:HA	1:A:640:ALA:HB2	1.73	0.68
1:A:5:VAL:HG22	1:A:6:GLU:H	1.58	0.68
1:A:321:TYR:O	1:A:322:VAL:HG22	1.93	0.68
1:A:191:ASP:HA	1:A:265:LYS:O	1.93	0.68
1:A:580:MET:O	1:A:584:ILE:HD13	1.93	0.68
1:A:239:GLU:O	1:A:243:VAL:HG23	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD21	1:A:303:PRO:CB	2.23	0.68
1:A:409:ILE:O	1:A:411:VAL:N	2.27	0.68
1:A:493:VAL:HG23	1:A:512:ILE:HG13	1.76	0.68
1:A:185:ALA:HB3	1:A:199:ILE:CG1	2.24	0.67
1:A:416:LYS:HG2	1:A:449:THR:HB	1.76	0.67
1:A:90:PHE:CE2	1:A:458:HIS:HA	2.30	0.67
1:A:438:PHE:O	1:A:439:ARG:HG3	1.93	0.67
1:A:504:ARG:HG2	1:A:504:ARG:HH11	1.60	0.66
1:A:396:ARG:HE	1:A:396:ARG:H	1.43	0.66
1:A:607:ARG:NH1	1:A:672:PHE:HB2	2.10	0.66
1:A:679:VAL:HG13	1:A:683:VAL:HB	1.77	0.66
1:A:614:GLU:OE1	1:A:641:GLN:HG3	1.96	0.66
1:A:466:LEU:O	1:A:468:ARG:N	2.29	0.65
1:A:413:ILE:HD12	1:A:459:LEU:HD11	1.78	0.65
1:A:92:ILE:HD13	1:A:92:ILE:H	1.59	0.65
1:A:14:ASN:HD22	1:A:329:ARG:HH21	1.44	0.65
1:A:357:ARG:HH11	1:A:357:ARG:CG	2.11	0.64
1:A:462:ILE:O	1:A:466:LEU:HB2	1.96	0.64
1:A:70:THR:HG22	1:A:71:THR:H	1.62	0.64
1:A:528:ALA:HB3	1:A:568:TYR:CA	2.26	0.64
1:A:443:HIS:O	1:A:448:GLN:N	2.30	0.64
1:A:147:TRP:O	1:A:151:ARG:HB2	1.98	0.64
1:A:309:LEU:HG	1:A:310:ALA:H	1.60	0.64
1:A:14:ASN:HD22	1:A:329:ARG:NH2	1.96	0.64
1:A:627:ARG:O	1:A:647:VAL:HG23	1.98	0.64
1:A:348:ARG:CZ	1:A:382:GLU:HG3	2.28	0.63
1:A:621:ILE:HG22	1:A:621:ILE:O	1.98	0.63
1:A:459:LEU:H	1:A:459:LEU:HD12	1.64	0.63
1:A:90:PHE:HE2	1:A:458:HIS:CA	2.12	0.63
1:A:115:GLU:HG2	1:A:118:SER:OG	1.99	0.62
1:A:27:THR:HG22	1:A:31:ARG:HG2	1.81	0.62
1:A:34:TYR:O	1:A:34:TYR:HD1	1.82	0.62
1:A:517:LEU:HD23	1:A:518:PRO:HD2	1.80	0.62
1:A:427:ALA:HA	1:A:470:PHE:CE2	2.34	0.62
1:A:97:SER:O	1:A:101:LEU:HD22	1.99	0.62
1:A:168:ILE:HD11	1:A:178:ILE:HD11	1.81	0.62
1:A:439:ARG:CB	1:A:439:ARG:NH1	2.63	0.61
1:A:458:HIS:HA	1:A:461:ILE:HG13	1.82	0.61
1:A:526:VAL:HG12	1:A:527:ASN:N	2.15	0.61
1:A:555:LEU:HD11	1:A:599:PRO:HB2	1.81	0.61
1:A:467:LYS:HG2	1:A:467:LYS:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HH22	1:A:381:LYS:HE3	1.64	0.61
1:A:468:ARG:HA	1:A:468:ARG:CZ	2.31	0.60
1:A:499:ARG:HG3	1:A:499:ARG:NH1	2.15	0.60
1:A:232:LEU:O	1:A:233:GLU:HB2	2.01	0.60
1:A:295:GLU:HG3	1:A:295:GLU:O	2.02	0.60
1:A:355:LEU:HD23	1:A:377:VAL:HA	1.83	0.60
1:A:71:THR:O	1:A:72:CYS:HB2	2.01	0.60
1:A:19:ALA:HB2	1:A:107:VAL:CG1	2.31	0.60
1:A:129:LYS:HG2	1:A:253:LEU:HD11	1.82	0.59
1:A:9:LEU:CD2	1:A:303:PRO:HB2	2.27	0.59
1:A:34:TYR:CD1	1:A:34:TYR:C	2.75	0.59
1:A:616:TYR:CD2	1:A:663:THR:HB	2.36	0.59
1:A:87:HIS:CE1	1:A:90:PHE:HB2	2.36	0.59
1:A:457:LEU:CG	1:A:460:GLU:HB2	2.26	0.59
1:A:517:LEU:HD22	1:A:521:SER:HB3	1.85	0.59
1:A:34:TYR:O	1:A:34:TYR:CD1	2.55	0.59
1:A:454:MET:HG2	1:A:455:GLY:H	1.68	0.59
1:A:413:ILE:CD1	1:A:459:LEU:HD11	2.31	0.59
1:A:497:PHE:O	1:A:498:ILE:HD12	2.02	0.59
1:A:546:ILE:HD13	1:A:565:VAL:HG11	1.84	0.59
1:A:628:ARG:HH11	1:A:648:PRO:HB2	1.67	0.59
1:A:91:THR:HA	1:A:94:VAL:HB	1.84	0.59
1:A:265:LYS:HB3	1:A:267:LYS:HZ3	1.67	0.59
1:A:153:MET:HE2	1:A:161:PRO:HB3	1.84	0.59
1:A:356:LEU:HD23	1:A:365:GLU:HA	1.83	0.59
1:A:681:LYS:N	1:A:681:LYS:CD	2.66	0.59
1:A:294:PRO:HD3	1:A:398:ILE:HD11	1.84	0.59
1:A:309:LEU:HA	1:A:332:SER:O	2.03	0.58
1:A:468:ARG:HH11	1:A:468:ARG:HG2	1.67	0.58
1:A:647:VAL:CG1	1:A:652:MET:SD	2.91	0.58
1:A:188:TYR:CE2	1:A:268:GLY:N	2.70	0.58
1:A:639:ASN:OD1	1:A:640:ALA:N	2.36	0.58
1:A:481:VAL:HG22	1:A:649:LEU:HD13	1.86	0.58
1:A:177:ILE:HD12	1:A:188:TYR:HE2	1.67	0.58
1:A:497:PHE:CG	1:A:584:ILE:HG21	2.39	0.58
1:A:433:GLU:HB3	1:A:434:GLU:OE1	2.02	0.58
1:A:498:ILE:HD11	1:A:507:TYR:CE2	2.39	0.58
1:A:684:GLN:O	1:A:688:ILE:HG12	2.03	0.58
1:A:204:GLU:N	1:A:204:GLU:OE1	2.37	0.58
1:A:78:ARG:CZ	1:A:357:ARG:HH21	2.17	0.58
1:A:342:TYR:CD1	1:A:348:ARG:O	2.57	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:O	1:A:76:ASP:HB3	2.03	0.57
1:A:160:ARG:CG	1:A:160:ARG:HH11	2.18	0.57
1:A:329:ARG:HH11	1:A:329:ARG:HG2	1.69	0.57
1:A:343:ASN:OD1	1:A:346:LYS:HB2	2.03	0.57
1:A:342:TYR:CE1	1:A:347:GLY:O	2.58	0.57
1:A:442:THR:O	1:A:448:GLN:N	2.38	0.57
1:A:681:LYS:H	1:A:681:LYS:HD2	1.70	0.57
1:A:165:GLN:HG3	1:A:260:LEU:HD13	1.87	0.57
1:A:196:ILE:O	1:A:196:ILE:HG12	2.04	0.56
1:A:454:MET:HB3	1:A:458:HIS:CD2	2.40	0.56
1:A:624:LEU:HD23	1:A:631:ILE:CD1	2.34	0.56
1:A:164:MET:CE	1:A:246:ILE:HG21	2.35	0.56
1:A:218:GLU:HG3	1:A:231:TYR:CE2	2.40	0.56
1:A:661:SER:OG	1:A:662:LYS:HD3	2.05	0.56
1:A:109:ASP:OD1	1:A:138:LYS:HD2	2.05	0.56
1:A:427:ALA:HA	1:A:470:PHE:CD2	2.41	0.56
1:A:427:ALA:CB	1:A:470:PHE:HD2	2.18	0.56
1:A:181:LEU:HD21	1:A:243:VAL:HG22	1.88	0.56
1:A:498:ILE:HD11	1:A:507:TYR:CD2	2.41	0.55
1:A:556:ILE:HD13	1:A:601:ILE:HD13	1.88	0.55
1:A:32:ILE:HG22	1:A:33:LEU:N	2.21	0.55
1:A:416:LYS:HA	1:A:449:THR:O	2.07	0.55
1:A:469:GLU:O	1:A:470:PHE:HD1	1.88	0.55
1:A:98:MET:HA	1:A:101:LEU:CD2	2.36	0.55
1:A:119:GLU:O	1:A:122:TRP:HB3	2.05	0.55
1:A:345:THR:HG23	1:A:388:THR:H	1.70	0.55
1:A:605:ILE:HD13	1:A:677:GLN:HB3	1.89	0.55
1:A:439:ARG:HB3	1:A:439:ARG:NH1	2.21	0.55
1:A:512:ILE:HG12	1:A:589:ALA:HB1	1.89	0.55
1:A:486:THR:HG22	1:A:487:ILE:O	2.06	0.55
1:A:491:VAL:HG11	1:A:596:LYS:O	2.07	0.55
1:A:188:TYR:CD2	1:A:267:LYS:HA	2.41	0.55
1:A:335:LEU:HD11	1:A:352:VAL:HG21	1.87	0.55
1:A:286:ILE:HG22	1:A:287:PRO:N	2.22	0.55
1:A:523:PHE:CD1	1:A:524:GLU:N	2.75	0.55
1:A:22:ASP:O	1:A:24:GLY:N	2.40	0.54
1:A:342:TYR:HE1	1:A:347:GLY:O	1.90	0.54
1:A:342:TYR:HD1	1:A:348:ARG:O	1.90	0.54
1:A:608:VAL:HG21	1:A:652:MET:HE2	1.90	0.54
1:A:341:VAL:HG23	1:A:350:GLU:HB2	1.87	0.54
1:A:646:PHE:O	1:A:648:PRO:HD3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ILE:HD11	1:A:369:LEU:HD11	1.89	0.54
1:A:415:PRO:HD2	1:A:451:ILE:O	2.07	0.54
1:A:496:LYS:HG3	1:A:509:HIS:HD1	1.72	0.54
1:A:539:ILE:CB	1:A:540:PRO:HD3	2.38	0.54
1:A:511:LYS:CD	1:A:569:ASP:HB3	2.36	0.54
1:A:90:PHE:CE2	1:A:458:HIS:CA	2.90	0.54
1:A:484:ARG:O	1:A:485:GLU:HG2	2.07	0.54
1:A:572:TYR:HB3	1:A:582:PHE:HZ	1.73	0.54
1:A:272:LEU:O	1:A:276:VAL:HG23	2.08	0.54
1:A:69:VAL:CG2	1:A:314:PHE:HZ	2.20	0.54
1:A:107:VAL:HG23	1:A:137:ASN:HB2	1.89	0.54
1:A:431:LEU:O	1:A:438:PHE:HE2	1.89	0.54
1:A:610:VAL:HG22	1:A:669:PHE:HB3	1.90	0.54
1:A:488:THR:OG1	1:A:598:ASP:HB2	2.07	0.54
1:A:616:TYR:OH	1:A:664:GLN:NE2	2.41	0.54
1:A:22:ASP:C	1:A:24:GLY:N	2.60	0.53
1:A:81:ILE:HG22	1:A:81:ILE:O	2.08	0.53
1:A:411:VAL:HB	1:A:453:GLY:HA2	1.91	0.53
1:A:460:GLU:O	1:A:463:VAL:HB	2.08	0.53
1:A:265:LYS:HB3	1:A:267:LYS:NZ	2.23	0.53
1:A:31:ARG:HD2	1:A:31:ARG:N	2.23	0.53
1:A:368:GLU:HG3	1:A:368:GLU:O	2.09	0.53
1:A:70:THR:HG22	1:A:71:THR:N	2.24	0.53
1:A:340:TYR:HB2	1:A:392:GLU:OE2	2.09	0.53
1:A:292:THR:O	1:A:398:ILE:HD12	2.09	0.53
1:A:290:LYS:HB3	1:A:298:VAL:CG1	2.37	0.53
1:A:78:ARG:NH2	1:A:357:ARG:HH21	2.07	0.53
1:A:343:ASN:ND2	1:A:383:THR:OG1	2.41	0.53
1:A:460:GLU:HA	1:A:463:VAL:CG2	2.39	0.52
1:A:609:GLU:O	1:A:669:PHE:HA	2.10	0.52
1:A:345:THR:OG1	1:A:387:ASP:OD1	2.27	0.52
1:A:377:VAL:O	1:A:377:VAL:HG22	2.08	0.52
1:A:465:ARG:HA	1:A:469:GLU:CB	2.39	0.52
1:A:608:VAL:HG12	1:A:610:VAL:HG23	1.91	0.52
1:A:276:VAL:CG1	1:A:280:LEU:HD12	2.38	0.52
1:A:608:VAL:HG21	1:A:652:MET:CE	2.39	0.52
1:A:572:TYR:N	1:A:572:TYR:CD1	2.76	0.52
1:A:187:THR:HG23	1:A:187:THR:O	2.10	0.52
1:A:457:LEU:HA	1:A:460:GLU:H	1.74	0.52
1:A:462:ILE:HG22	1:A:466:LEU:HD13	1.91	0.52
1:A:465:ARG:HA	1:A:469:GLU:HB3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LEU:HD22	1:A:521:SER:CB	2.40	0.52
1:A:624:LEU:CD2	1:A:631:ILE:HD11	2.38	0.52
1:A:610:VAL:HG22	1:A:669:PHE:CB	2.39	0.52
1:A:643:ILE:HG12	1:A:643:ILE:O	2.10	0.52
1:A:87:HIS:O	1:A:89:ASP:N	2.43	0.52
1:A:398:ILE:H	1:A:398:ILE:HD12	1.74	0.51
1:A:227:ILE:HG23	1:A:237:PRO:HG2	1.93	0.51
1:A:497:PHE:CD1	1:A:584:ILE:HG21	2.46	0.51
1:A:661:SER:OG	1:A:662:LYS:N	2.44	0.51
1:A:25:LYS:NZ	1:A:84:THR:OG1	2.43	0.51
1:A:315:LYS:O	1:A:327:PHE:HB2	2.10	0.51
1:A:526:VAL:CG1	1:A:527:ASN:N	2.74	0.51
1:A:514:VAL:CG2	1:A:593:ALA:HB1	2.38	0.51
1:A:329:ARG:HG2	1:A:331:TYR:CZ	2.45	0.51
1:A:608:VAL:CG1	1:A:610:VAL:HG23	2.41	0.51
1:A:613:PRO:O	1:A:615:GLU:N	2.43	0.51
1:A:430:ARG:C	1:A:432:ALA:H	2.14	0.51
1:A:624:LEU:HD23	1:A:631:ILE:CG1	2.41	0.51
1:A:246:ILE:O	1:A:246:ILE:HG22	2.11	0.51
1:A:348:ARG:NE	1:A:382:GLU:HG3	2.25	0.51
1:A:98:MET:HA	1:A:101:LEU:HD22	1.91	0.51
1:A:528:ALA:N	1:A:567:LEU:O	2.43	0.51
1:A:577:SER:HB3	1:A:582:PHE:CE1	2.41	0.50
1:A:685:GLU:HA	1:A:688:ILE:HD11	1.93	0.50
1:A:411:VAL:HG21	1:A:439:ARG:HD3	1.93	0.50
1:A:555:LEU:CD1	1:A:599:PRO:HB2	2.41	0.50
1:A:170:ARG:N	1:A:173:THR:HB	2.23	0.50
1:A:514:VAL:HG21	1:A:593:ALA:CB	2.41	0.50
1:A:179:ASP:OD2	1:A:182:ARG:HB2	2.11	0.50
1:A:457:LEU:C	1:A:459:LEU:N	2.63	0.50
1:A:603:GLU:HB2	1:A:604:PRO:HD2	1.93	0.50
1:A:620:VAL:C	1:A:622:GLY:H	2.15	0.50
1:A:256:THR:O	1:A:256:THR:HG22	2.12	0.50
1:A:329:ARG:CD	1:A:374:LEU:HD23	2.41	0.50
1:A:573:HIS:HB3	1:A:576:ASP:H	1.76	0.50
1:A:607:ARG:HA	1:A:645:ALA:O	2.12	0.50
1:A:140:ASP:HA	1:A:171:GLU:HA	1.94	0.50
1:A:671:MET:O	1:A:672:PHE:HD1	1.94	0.50
1:A:357:ARG:NH1	1:A:357:ARG:CG	2.68	0.50
1:A:361:ASN:O	1:A:362:HIS:CB	2.59	0.50
1:A:110:SER:HB2	1:A:137:ASN:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.25	0.49
1:A:572:TYR:HD1	1:A:572:TYR:O	1.95	0.49
1:A:413:ILE:HA	1:A:480:GLN:O	2.12	0.49
1:A:361:ASN:O	1:A:362:HIS:HB3	2.10	0.49
1:A:519:ARG:HB2	1:A:519:ARG:NH1	2.25	0.49
1:A:530:VAL:O	1:A:530:VAL:HG23	2.12	0.49
1:A:377:VAL:HG22	1:A:380:LEU:HD12	1.93	0.49
1:A:500:GLN:O	1:A:502:GLY:N	2.46	0.49
1:A:554:PRO:HB3	1:A:595:GLN:HE21	1.76	0.49
1:A:443:HIS:HB2	1:A:450:ILE:HD13	1.95	0.49
1:A:434:GLU:N	1:A:434:GLU:OE1	2.45	0.49
1:A:517:LEU:CD2	1:A:518:PRO:HD2	2.43	0.49
1:A:604:PRO:HG2	1:A:649:LEU:HB3	1.95	0.49
1:A:411:VAL:O	1:A:453:GLY:HA2	2.12	0.49
1:A:558:PHE:HB3	1:A:559:PRO:HD2	1.94	0.49
1:A:269:VAL:HG23	1:A:270:GLN:OE1	2.13	0.49
1:A:301:ILE:HG23	1:A:332:SER:HB2	1.93	0.49
1:A:119:GLU:HG3	1:A:157:LEU:HD12	1.94	0.49
1:A:344:THR:HG22	1:A:396:ARG:HB2	1.95	0.49
1:A:450:ILE:O	1:A:450:ILE:HG13	2.13	0.49
1:A:182:ARG:O	1:A:183:MET:HB2	2.13	0.48
1:A:344:THR:HG21	1:A:397:VAL:N	2.27	0.48
1:A:348:ARG:NH2	1:A:382:GLU:HG3	2.28	0.48
1:A:357:ARG:NH1	1:A:357:ARG:HG3	2.20	0.48
1:A:500:GLN:C	1:A:502:GLY:N	2.67	0.48
1:A:607:ARG:HH11	1:A:672:PHE:HB2	1.76	0.48
1:A:19:ALA:HB2	1:A:107:VAL:HG12	1.96	0.48
1:A:438:PHE:CD1	1:A:439:ARG:N	2.82	0.48
1:A:547:GLU:HG2	1:A:547:GLU:O	2.14	0.48
1:A:553:GLY:O	1:A:557:GLY:HA2	2.12	0.48
1:A:156:ARG:NH1	1:A:666:ARG:HH11	2.11	0.48
1:A:329:ARG:HA	1:A:374:LEU:HB3	1.95	0.48
1:A:314:PHE:CD1	1:A:315:LYS:HB2	2.49	0.48
1:A:392:GLU:O	1:A:392:GLU:HG3	2.14	0.48
1:A:20:HIS:NE2	1:A:21:ILE:HG13	2.29	0.48
1:A:162:VAL:HG12	1:A:163:VAL:N	2.28	0.48
1:A:188:TYR:OH	1:A:271:LEU:HD12	2.14	0.48
1:A:415:PRO:O	1:A:450:ILE:HA	2.13	0.48
1:A:544:LYS:HZ3	1:A:583:LYS:HZ3	1.62	0.48
1:A:92:ILE:HG12	1:A:92:ILE:O	2.12	0.48
1:A:171:GLU:CG	1:A:172:ASP:H	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HD3	1:A:331:TYR:OH	2.13	0.47
1:A:528:ALA:HB3	1:A:567:LEU:O	2.14	0.47
1:A:227:ILE:HG23	1:A:237:PRO:CG	2.44	0.47
1:A:542:VAL:O	1:A:544:LYS:N	2.47	0.47
1:A:554:PRO:HG2	1:A:594:VAL:HB	1.96	0.47
1:A:329:ARG:CG	1:A:329:ARG:HH11	2.26	0.47
1:A:286:ILE:CG2	1:A:287:PRO:N	2.78	0.47
1:A:20:HIS:ND1	1:A:117:GLN:OE1	2.47	0.47
1:A:243:VAL:HG13	1:A:279:TYR:CE1	2.50	0.47
1:A:319:ASP:CG	1:A:363:ARG:HH22	2.18	0.47
1:A:493:VAL:HG23	1:A:512:ILE:CG1	2.43	0.47
1:A:114:VAL:O	1:A:114:VAL:HG12	2.13	0.47
1:A:168:ILE:HD11	1:A:178:ILE:CD1	2.44	0.47
1:A:91:THR:O	1:A:94:VAL:N	2.48	0.47
1:A:153:MET:HA	1:A:157:LEU:HD22	1.96	0.47
1:A:616:TYR:O	1:A:618:GLY:N	2.45	0.47
1:A:319:ASP:HB3	1:A:322:VAL:HG22	1.97	0.47
1:A:367:GLU:O	1:A:368:GLU:HB3	2.15	0.47
1:A:343:ASN:OD1	1:A:346:LYS:N	2.48	0.47
1:A:506:GLN:HA	1:A:576:ASP:O	2.15	0.47
1:A:672:PHE:N	1:A:672:PHE:CD1	2.82	0.47
1:A:410:ASP:O	1:A:411:VAL:HG22	2.15	0.47
1:A:637:ARG:HH11	1:A:637:ARG:HG2	1.80	0.47
1:A:671:MET:C	1:A:672:PHE:CD1	2.78	0.47
1:A:120:THR:HG21	1:A:668:SER:HB3	1.96	0.47
1:A:140:ASP:HB3	1:A:174:PHE:HD2	1.79	0.47
1:A:465:ARG:CA	1:A:469:GLU:HB3	2.45	0.46
1:A:630:GLN:O	1:A:631:ILE:C	2.51	0.46
1:A:328:ILE:HG12	1:A:377:VAL:HG12	1.97	0.46
1:A:613:PRO:HG3	1:A:666:ARG:HH21	1.79	0.46
1:A:8:ASP:HB3	1:A:11:ARG:HG2	1.97	0.46
1:A:90:PHE:CE2	1:A:461:ILE:HD11	2.50	0.46
1:A:309:LEU:CG	1:A:310:ALA:N	2.75	0.46
1:A:319:ASP:CG	1:A:363:ARG:HH12	2.19	0.46
1:A:534:ILE:HD11	1:A:570:GLY:HA3	1.98	0.46
1:A:523:PHE:CD1	1:A:550:MET:HE1	2.51	0.46
1:A:614:GLU:H	1:A:614:GLU:HG2	1.53	0.46
1:A:627:ARG:HA	1:A:651:GLU:HG2	1.98	0.46
1:A:300:GLU:HG2	1:A:302:HIS:HE1	1.81	0.46
1:A:354:ARG:HG3	1:A:378:VAL:HG12	1.98	0.46
1:A:499:ARG:HG3	1:A:501:THR:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:TYR:CD1	1:A:572:TYR:O	2.68	0.46
1:A:573:HIS:ND1	1:A:576:ASP:HB2	2.30	0.46
1:A:329:ARG:NH1	1:A:331:TYR:CE1	2.84	0.46
1:A:176:GLY:CA	1:A:187:THR:HA	2.44	0.46
1:A:294:PRO:O	1:A:295:GLU:HB3	2.16	0.46
1:A:416:LYS:HG2	1:A:449:THR:CB	2.45	0.46
1:A:608:VAL:HG12	1:A:609:GLU:N	2.31	0.46
1:A:133:ILE:HD12	1:A:259:PHE:CE2	2.51	0.46
1:A:160:ARG:CG	1:A:160:ARG:NH1	2.77	0.46
1:A:185:ALA:HB3	1:A:199:ILE:HG12	1.97	0.46
1:A:620:VAL:O	1:A:624:LEU:HB2	2.17	0.45
1:A:146:LEU:HD12	1:A:167:PRO:HD2	1.98	0.45
1:A:357:ARG:HD3	1:A:364:GLU:OE2	2.16	0.45
1:A:512:ILE:CD1	1:A:589:ALA:HB1	2.46	0.45
1:A:357:ARG:O	1:A:359:HIS:HD2	1.99	0.45
1:A:628:ARG:CD	1:A:648:PRO:HG2	2.41	0.45
1:A:38:ARG:CG	1:A:39:ILE:H	2.29	0.45
1:A:416:LYS:HG2	1:A:449:THR:CG2	2.46	0.45
1:A:490:PRO:HG3	1:A:516:PRO:HD3	1.98	0.45
1:A:672:PHE:N	1:A:672:PHE:HD1	2.14	0.45
1:A:584:ILE:HG22	1:A:585:ALA:N	2.32	0.45
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.59	0.45
1:A:102:ASP:HB3	1:A:286:ILE:HD11	1.97	0.45
1:A:270:GLN:O	1:A:273:LEU:N	2.47	0.45
1:A:430:ARG:C	1:A:432:ALA:N	2.68	0.45
1:A:435:ASP:C	1:A:437:THR:H	2.19	0.45
1:A:518:PRO:HB2	1:A:521:SER:OG	2.16	0.45
1:A:605:ILE:HG13	1:A:648:PRO:HG3	1.98	0.45
1:A:688:ILE:O	1:A:689:LYS:HD3	2.16	0.45
1:A:85:PRO:HG3	1:A:94:VAL:CA	2.39	0.45
1:A:90:PHE:O	1:A:94:VAL:HG23	2.17	0.45
1:A:238:THR:OG1	1:A:241:GLU:HB2	2.17	0.45
1:A:269:VAL:O	1:A:270:GLN:C	2.55	0.45
1:A:364:GLU:O	1:A:364:GLU:HG2	2.17	0.45
1:A:544:LYS:NZ	1:A:583:LYS:NZ	2.63	0.45
1:A:674:ASP:O	1:A:675:HIS:HB3	2.17	0.45
1:A:69:VAL:HG21	1:A:314:PHE:HZ	1.81	0.45
1:A:536:LYS:HA	1:A:539:ILE:HD12	1.99	0.45
1:A:613:PRO:HG3	1:A:666:ARG:HE	1.82	0.45
1:A:627:ARG:HB3	1:A:647:VAL:HG21	1.98	0.45
1:A:553:GLY:HA2	1:A:554:PRO:HD3	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LEU:HA	1:A:659:LEU:HD12	1.76	0.44
1:A:500:GLN:C	1:A:502:GLY:H	2.21	0.44
1:A:632:LEU:HG	1:A:633:GLY:N	2.32	0.44
1:A:146:LEU:HD12	1:A:167:PRO:CD	2.48	0.44
1:A:361:ASN:O	1:A:362:HIS:ND1	2.50	0.44
1:A:409:ILE:C	1:A:411:VAL:H	2.20	0.44
1:A:129:LYS:O	1:A:129:LYS:CD	2.65	0.44
1:A:427:ALA:O	1:A:429:ALA:N	2.51	0.44
1:A:539:ILE:O	1:A:543:GLN:HG3	2.18	0.44
1:A:687:LEU:HA	1:A:687:LEU:HD23	1.77	0.44
1:A:129:LYS:O	1:A:129:LYS:CG	2.65	0.44
1:A:465:ARG:C	1:A:469:GLU:HB3	2.38	0.44
1:A:538:TYR:O	1:A:541:ALA:N	2.51	0.44
1:A:16:GLY:HA3	1:A:101:LEU:HD12	1.99	0.44
1:A:186:TYR:CE1	1:A:198:GLU:HG2	2.53	0.43
1:A:604:PRO:O	1:A:649:LEU:HB2	2.18	0.43
1:A:114:VAL:O	1:A:156:ARG:NH2	2.51	0.43
1:A:119:GLU:OE2	1:A:123:ARG:NH1	2.52	0.43
1:A:162:VAL:CG1	1:A:163:VAL:N	2.82	0.43
1:A:176:GLY:HA2	1:A:186:TYR:O	2.19	0.43
1:A:288:PRO:HB2	1:A:300:GLU:HG3	1.99	0.43
1:A:477:GLY:C	1:A:479:PRO:HD3	2.38	0.43
1:A:651:GLU:O	1:A:652:MET:HB2	2.18	0.43
1:A:199:ILE:HB	1:A:200:PRO:HD2	2.00	0.43
1:A:22:ASP:O	1:A:23:ALA:C	2.55	0.43
1:A:579:GLU:O	1:A:581:ALA:N	2.50	0.43
1:A:621:ILE:CG2	1:A:621:ILE:O	2.65	0.43
1:A:146:LEU:O	1:A:149:VAL:HB	2.18	0.43
1:A:20:HIS:CD2	1:A:21:ILE:HG13	2.54	0.43
1:A:427:ALA:HB2	1:A:470:PHE:HD2	1.82	0.43
1:A:535:PRO:O	1:A:537:GLU:N	2.52	0.43
1:A:5:VAL:CG2	1:A:6:GLU:N	2.78	0.43
1:A:11:ARG:H	1:A:11:ARG:HG2	1.63	0.43
1:A:354:ARG:HG3	1:A:378:VAL:CG1	2.49	0.43
1:A:391:GLY:H	1:A:394:ALA:HB3	1.83	0.43
1:A:431:LEU:O	1:A:438:PHE:CE2	2.70	0.43
1:A:156:ARG:HH11	1:A:666:ARG:HH11	1.66	0.43
1:A:344:THR:HG1	1:A:388:THR:HB	1.81	0.43
1:A:477:GLY:O	1:A:479:PRO:HD3	2.18	0.43
1:A:519:ARG:HA	1:A:562:ASP:OD2	2.19	0.43
1:A:664:GLN:O	1:A:666:ARG:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:GLU:HA	1:A:688:ILE:CD1	2.49	0.43
1:A:215:LYS:O	1:A:218:GLU:HB3	2.19	0.43
1:A:443:HIS:HA	1:A:444:PRO:HD3	1.51	0.43
1:A:500:GLN:HA	1:A:500:GLN:OE1	2.19	0.43
1:A:631:ILE:H	1:A:631:ILE:HD12	1.83	0.43
1:A:22:ASP:C	1:A:24:GLY:H	2.21	0.43
1:A:27:THR:HG22	1:A:31:ARG:CG	2.48	0.43
1:A:671:MET:O	1:A:672:PHE:CD1	2.72	0.43
1:A:120:THR:O	1:A:123:ARG:HB2	2.18	0.42
1:A:12:LEU:O	1:A:283:PRO:HD3	2.19	0.42
1:A:251:ILE:HG23	1:A:281:PRO:HB3	2.01	0.42
1:A:350:GLU:OE1	1:A:380:LEU:HD23	2.19	0.42
1:A:493:VAL:CG2	1:A:593:ALA:HB2	2.41	0.42
1:A:111:SER:OG	1:A:141:LYS:HD3	2.18	0.42
1:A:141:LYS:O	1:A:142:THR:C	2.57	0.42
1:A:21:ILE:HB	1:A:22:ASP:H	1.65	0.42
1:A:469:GLU:C	1:A:470:PHE:HD1	2.23	0.42
1:A:156:ARG:HH11	1:A:666:ARG:NH1	2.17	0.42
1:A:572:TYR:C	1:A:572:TYR:CD1	2.90	0.42
1:A:150:ILE:HG12	1:A:150:ILE:H	1.73	0.42
1:A:186:TYR:HE1	1:A:198:GLU:HG2	1.85	0.42
1:A:590:ILE:HD13	1:A:590:ILE:HA	1.77	0.42
1:A:227:ILE:HD11	1:A:241:GLU:HB3	2.01	0.42
1:A:327:PHE:CE1	1:A:376:ALA:HB2	2.55	0.42
1:A:655:TYR:O	1:A:655:TYR:CD1	2.72	0.42
1:A:359:HIS:NE2	1:A:364:GLU:HB3	2.35	0.42
1:A:129:LYS:O	1:A:129:LYS:HD3	2.19	0.42
1:A:561:VAL:O	1:A:563:ILE:HG23	2.20	0.42
1:A:654:GLY:O	1:A:656:ALA:N	2.53	0.42
1:A:679:VAL:CG1	1:A:683:VAL:HB	2.46	0.42
1:A:354:ARG:CG	1:A:378:VAL:CG1	2.98	0.42
1:A:38:ARG:HG3	1:A:39:ILE:H	1.85	0.42
1:A:90:PHE:CD2	1:A:461:ILE:HD11	2.54	0.42
1:A:572:TYR:HD1	1:A:572:TYR:H	1.65	0.41
1:A:636:PRO:CA	1:A:641:GLN:HG2	2.48	0.41
1:A:484:ARG:HG2	1:A:676:TYR:HE2	1.85	0.41
1:A:5:VAL:CG2	1:A:6:GLU:H	2.29	0.41
1:A:31:ARG:NH2	1:A:266:ASN:HD21	2.18	0.41
1:A:323:GLY:O	1:A:324:ARG:C	2.58	0.41
1:A:608:VAL:CG2	1:A:652:MET:HE2	2.50	0.41
1:A:674:ASP:OD2	1:A:675:HIS:ND1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:HD2	1:A:76:ASP:OD2	2.20	0.41
1:A:523:PHE:CE1	1:A:550:MET:HE1	2.55	0.41
1:A:669:PHE:HD1	1:A:669:PHE:H	1.69	0.41
1:A:588:MET:O	1:A:589:ALA:C	2.59	0.41
1:A:341:VAL:CG2	1:A:350:GLU:HB2	2.51	0.41
1:A:384:ILE:HB	1:A:385:THR:H	1.32	0.41
1:A:8:ASP:HB3	1:A:11:ARG:H	1.86	0.41
1:A:218:GLU:O	1:A:221:ALA:HB3	2.21	0.41
1:A:624:LEU:CG	1:A:631:ILE:HD11	2.50	0.41
1:A:165:GLN:HG3	1:A:260:LEU:CD1	2.48	0.41
1:A:18:ALA:O	1:A:106:VAL:HA	2.21	0.41
1:A:467:LYS:O	1:A:468:ARG:NH1	2.54	0.41
1:A:230:LYS:HB3	1:A:235:GLU:O	2.20	0.41
1:A:69:VAL:O	1:A:69:VAL:HG12	2.19	0.41
1:A:612:THR:CG2	1:A:663:THR:HG21	2.51	0.41
1:A:342:TYR:HE1	1:A:347:GLY:C	2.25	0.40
1:A:350:GLU:HB3	1:A:380:LEU:CD2	2.51	0.40
1:A:443:HIS:HB2	1:A:450:ILE:CD1	2.51	0.40
1:A:166:LEU:HD22	1:A:180:VAL:HG11	2.03	0.40
1:A:246:ILE:CG2	1:A:246:ILE:O	2.69	0.40
1:A:531:GLY:O	1:A:532:GLY:O	2.40	0.40
1:A:627:ARG:HB3	1:A:647:VAL:CG2	2.52	0.40
1:A:247:ARG:HD2	1:A:278:ASP:O	2.21	0.40
1:A:281:PRO:HA	1:A:285:ASP:OD2	2.21	0.40
1:A:296:GLY:O	1:A:297:GLU:CB	2.64	0.40
1:A:449:THR:O	1:A:450:ILE:CG2	2.69	0.40
1:A:542:VAL:O	1:A:543:GLN:C	2.60	0.40
1:A:87:HIS:CE1	1:A:90:PHE:CB	3.04	0.40
1:A:319:ASP:OD2	1:A:363:ARG:NH2	2.51	0.40
1:A:499:ARG:CG	1:A:499:ARG:NH1	2.76	0.40
1:A:542:VAL:C	1:A:544:LYS:N	2.74	0.40
1:A:602:LEU:HD12	1:A:602:LEU:HA	1.97	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	620/691 (90%)	437 (70%)	115 (18%)	68 (11%)	0 1

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	69	VAL
1	A	82	ILE
1	A	104	ALA
1	A	138	LYS
1	A	174	PHE
1	A	233	GLU
1	A	295	GLU
1	A	353	ALA
1	A	362	HIS
1	A	393	ASP
1	A	410	ASP
1	A	412	ALA
1	A	435	ASP
1	A	442	THR
1	A	443	HIS
1	A	454	MET
1	A	467	LYS
1	A	532	GLY
1	A	614	GLU
1	A	617	MET
1	A	649	LEU
1	A	652	MET
1	A	678	GLU
1	A	88	VAL
1	A	93	GLU
1	A	171	GLU
1	A	324	ARG
1	A	427	ALA
1	A	428	LEU
1	A	438	PHE
1	A	455	GLY
1	A	457	LEU
1	A	501	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	536	LYS
1	A	555	LEU
1	A	639	ASN
1	A	662	LYS
1	A	6	GLU
1	A	23	ALA
1	A	137	ASN
1	A	140	ASP
1	A	144	ALA
1	A	348	ARG
1	A	368	GLU
1	A	384	ILE
1	A	415	PRO
1	A	468	ARG
1	A	640	ALA
1	A	681	LYS
1	A	72	CYS
1	A	83	ASP
1	A	86	GLY
1	A	114	VAL
1	A	655	TYR
1	A	21	ILE
1	A	142	THR
1	A	478	LYS
1	A	580	MET
1	A	90	PHE
1	A	196	ILE
1	A	264	LEU
1	A	322	VAL
1	A	648	PRO
1	A	287	PRO
1	A	338	GLY
1	A	688	ILE
1	A	575	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	534/582 (92%)	409 (77%)	125 (23%)	1 2

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TYR
1	A	11	ARG
1	A	12	LEU
1	A	15	ILE
1	A	27	THR
1	A	34	TYR
1	A	36	THR
1	A	38	ARG
1	A	39	ILE
1	A	83	ASP
1	A	84	THR
1	A	85	PRO
1	A	87	HIS
1	A	92	ILE
1	A	93	GLU
1	A	96	ARG
1	A	99	ARG
1	A	101	LEU
1	A	110	SER
1	A	115	GLU
1	A	118	SER
1	A	123	ARG
1	A	129	LYS
1	A	132	ARG
1	A	137	ASN
1	A	151	ARG
1	A	157	LEU
1	A	166	LEU
1	A	175	SER
1	A	181	LEU
1	A	196	ILE
1	A	197	ARG
1	A	206	LEU
1	A	226	ASN
1	A	236	GLU
1	A	242	LEU
1	A	260	LEU
1	A	264	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	269	VAL
1	A	274	ASP
1	A	278	ASP
1	A	284	LEU
1	A	288	PRO
1	A	293	THR
1	A	294	PRO
1	A	297	GLU
1	A	300	GLU
1	A	302	HIS
1	A	309	LEU
1	A	312	LEU
1	A	321	TYR
1	A	322	VAL
1	A	326	THR
1	A	329	ARG
1	A	335	LEU
1	A	337	SER
1	A	348	ARG
1	A	352	VAL
1	A	357	ARG
1	A	365	GLU
1	A	367	GLU
1	A	369	LEU
1	A	370	LYS
1	A	374	LEU
1	A	377	VAL
1	A	378	VAL
1	A	381	LYS
1	A	383	THR
1	A	384	ILE
1	A	389	LEU
1	A	395	PRO
1	A	396	ARG
1	A	398	ILE
1	A	414	GLU
1	A	415	PRO
1	A	416	LYS
1	A	435	ASP
1	A	437	THR
1	A	440	VAL
1	A	452	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	458	HIS
1	A	464	ASP
1	A	466	LEU
1	A	468	ARG
1	A	480	GLN
1	A	492	ASP
1	A	506	GLN
1	A	514	VAL
1	A	518	PRO
1	A	519	ARG
1	A	550	MET
1	A	551	GLN
1	A	554	PRO
1	A	566	THR
1	A	569	ASP
1	A	572	TYR
1	A	575	VAL
1	A	579	GLU
1	A	580	MET
1	A	602	LEU
1	A	605	ILE
1	A	607	ARG
1	A	612	THR
1	A	614	GLU
1	A	619	ASP
1	A	621	ILE
1	A	623	ASP
1	A	625	ASN
1	A	632	LEU
1	A	634	MET
1	A	641	GLN
1	A	643	ILE
1	A	644	ARG
1	A	648	PRO
1	A	649	LEU
1	A	652	MET
1	A	660	ARG
1	A	664	GLN
1	A	669	PHE
1	A	670	VAL
1	A	679	VAL
1	A	681	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	682	GLN
1	A	683	VAL
1	A	689	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	208	GLN
1	A	302	HIS
1	A	343	ASN
1	A	426	GLN
1	A	595	GLN
1	A	625	ASN
1	A	664	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.