



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:34 am GMT

PDB ID : 4F52
Title : Structure of a Glomulin-RBX1-CUL1 complex
Authors : Duda, D.M.; Olszewski, J.L.; Schulman, B.A.
Deposited on : 2012-05-11
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

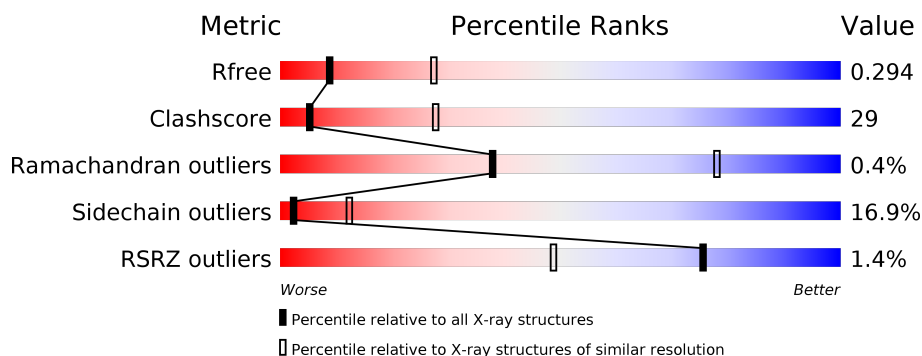
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	282	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>35%</div> <div>9%</div> <div>9%</div> </div> </div>
1	C	282	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>35%</div> <div>7%</div> <div>10%</div> </div> </div>
2	B	106	<div> <div>%</div> <div> <div></div> <div>36%</div> <div>40%</div> <div>•</div> <div>21%</div> </div> </div>
2	D	106	<div> <div></div> <div> <div></div> <div>37%</div> <div>33%</div> <div>10%</div> <div>20%</div> </div> </div>
3	E	596	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>39%</div> <div>8%</div> <div>12%</div> </div> </div>
3	F	596	<div> <div>%</div> <div> <div></div> <div>33%</div> <div>44%</div> <div>9%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13897 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 Cullin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2103	1341	351	400	11			
1	C	254	Total	C	N	O	S	0	0	0
			2073	1326	345	392	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	EXPRESSION TAG	UNP Q13616
A	410	SER	-	EXPRESSION TAG	UNP Q13616
A	421	GLU	LEU	ENGINEERED MUTATION	UNP Q13616
A	451	GLU	VAL	ENGINEERED MUTATION	UNP Q13616
A	452	LYS	VAL	ENGINEERED MUTATION	UNP Q13616
A	455	LYS	TYR	ENGINEERED MUTATION	UNP Q13616
C	409	GLY	-	EXPRESSION TAG	UNP Q13616
C	410	SER	-	EXPRESSION TAG	UNP Q13616
C	421	GLU	LEU	ENGINEERED MUTATION	UNP Q13616
C	451	GLU	VAL	ENGINEERED MUTATION	UNP Q13616
C	452	LYS	VAL	ENGINEERED MUTATION	UNP Q13616
C	455	LYS	TYR	ENGINEERED MUTATION	UNP Q13616

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	84	Total	C	N	O	S	0	0	0
			692	438	127	118	9			
2	D	85	Total	C	N	O	S	0	0	0
			701	443	128	121	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	-	EXPRESSION TAG	UNP P62877
B	4	SER	-	EXPRESSION TAG	UNP P62877
D	3	GLY	-	EXPRESSION TAG	UNP P62877
D	4	SER	-	EXPRESSION TAG	UNP P62877

- Molecule 3 is a protein called Glomulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	523	Total	C	N	O	S	0	0	0
			4202	2720	685	772	25			
3	F	512	Total	C	N	O	S	0	0	0
			4120	2676	666	753	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	EXPRESSION TAG	UNP Q92990
E	0	SER	-	EXPRESSION TAG	UNP Q92990
F	-1	GLY	-	EXPRESSION TAG	UNP Q92990
F	0	SER	-	EXPRESSION TAG	UNP Q92990

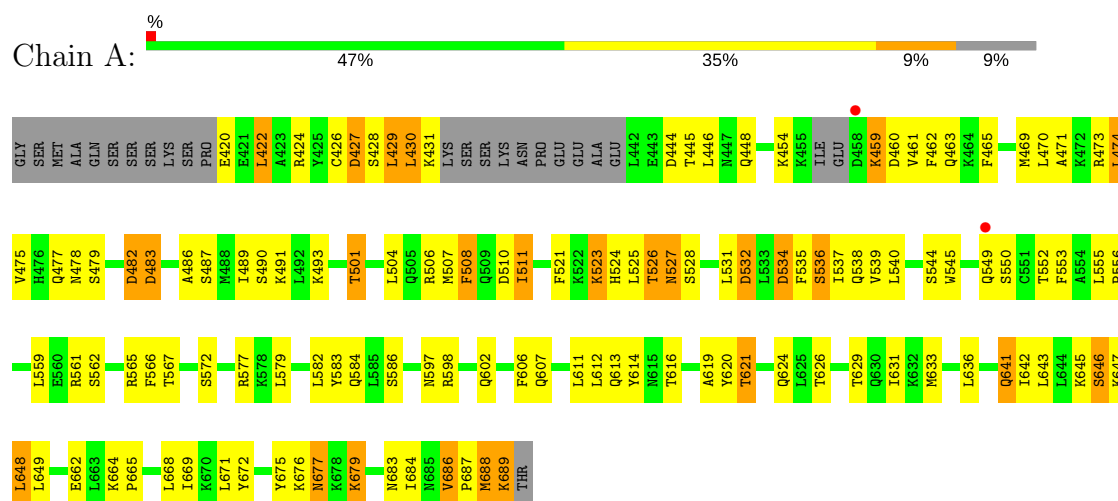
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Zn	0	0
			3	3		
4	D	3	Total	Zn	0	0
			3	3		

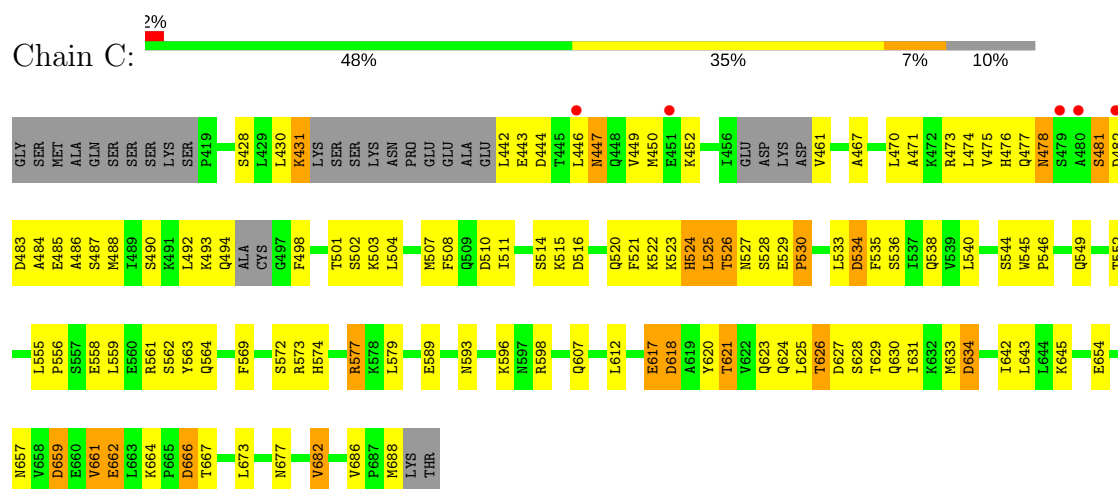
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

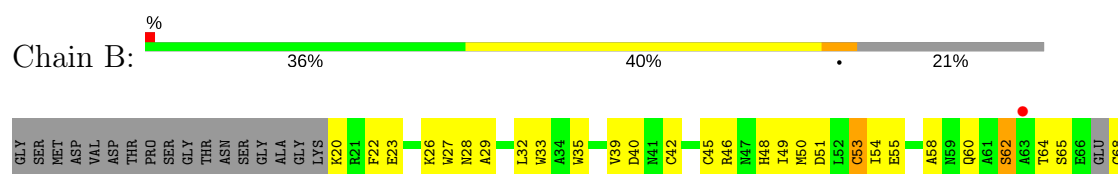
• Molecule 1: Cullin-1

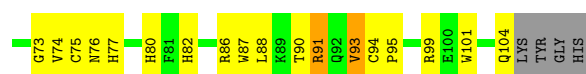


• Molecule 1: Cullin-1

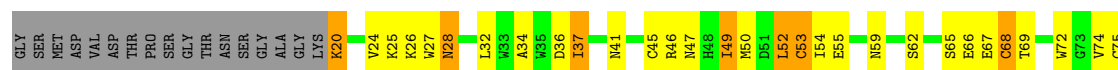


• Molecule 2: E3 ubiquitin-protein ligase RBX1

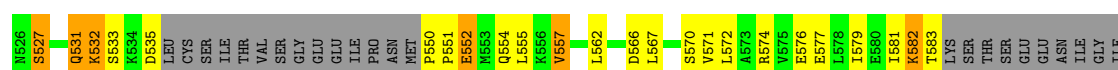
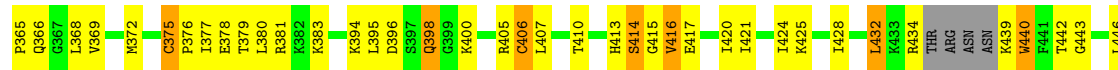
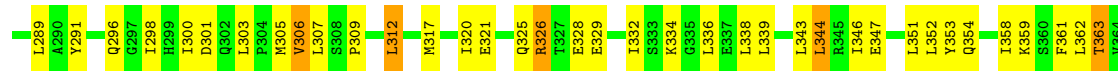
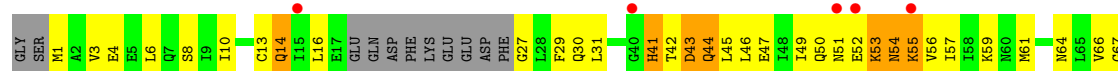




• Molecule 2: E3 ubiquitin-protein ligase RBX1

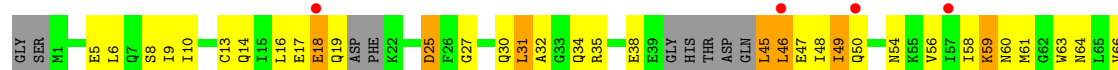


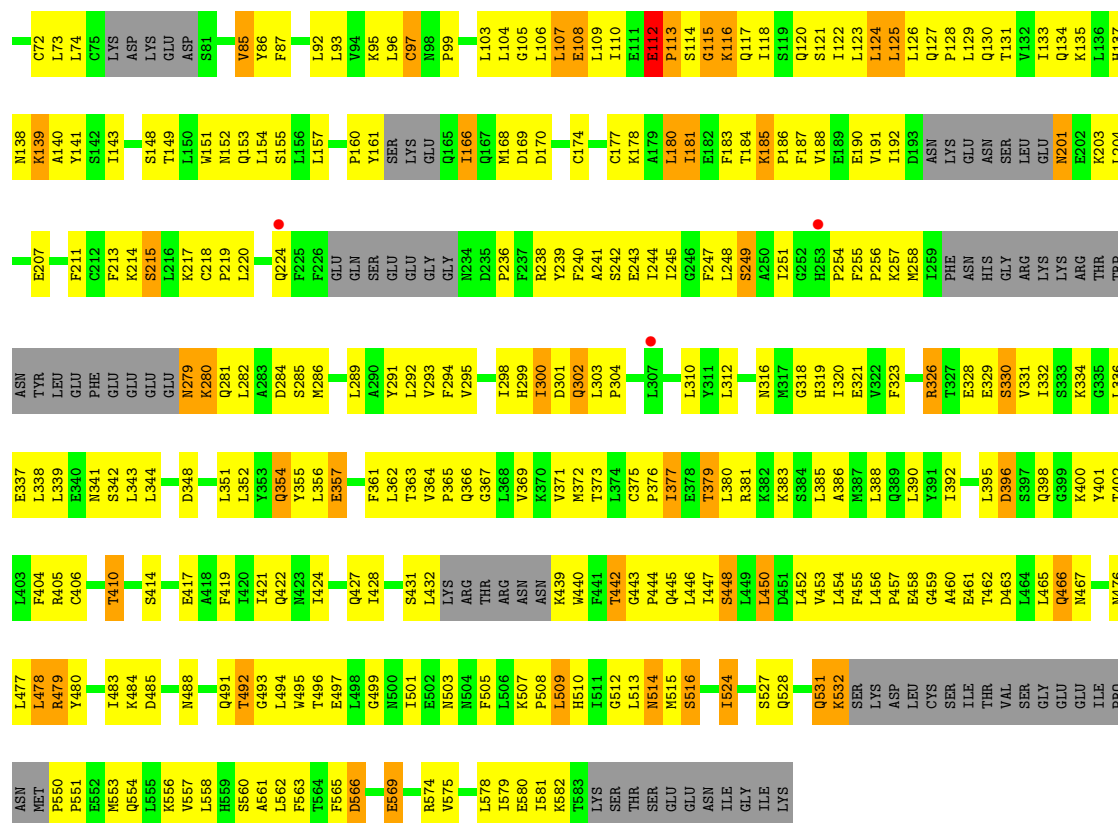
• Molecule 3: Glomulin



LYS

• Molecule 3: Glomulin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.33Å 193.93Å 142.07Å 90.00° 98.81° 90.00°	Depositor
Resolution (Å)	37.39 – 3.00 45.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.39-3.00) 98.8 (45.83-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.219 , 0.289 0.226 , 0.294	Depositor DCC
R_{free} test set	2831 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	83.5	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13897	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.46	0/2136	0.62	0/2870
1	C	0.43	0/2106	0.61	0/2830
2	B	0.47	0/711	0.68	0/965
2	D	0.44	0/721	0.66	0/980
3	E	0.44	0/4269	0.63	0/5753
3	F	0.39	0/4184	0.60	0/5639
All	All	0.43	0/14127	0.62	0/19037

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
3	E	0	4
3	F	0	4
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	501	THR	Peptide
3	E	111	GLU	Peptide
3	E	432	LEU	Peptide
3	E	492	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	E	493	GLY	Peptide
3	F	112	GLU	Peptide
3	F	114	SER	Peptide
3	F	115	GLY	Peptide
3	F	492	THR	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	2103	0	2127	117	0
1	C	2073	0	2101	118	0
2	B	692	0	647	48	0
2	D	701	0	654	44	0
3	E	4202	0	4360	271	0
3	F	4120	0	4271	277	0
4	B	3	0	0	0	0
4	D	3	0	0	0	0
All	All	13897	0	14160	820	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 29.

All (820) 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:C:525:LEU:O	1:C:529:GLU:HB2	1.21	1.37
1:C:530:PRO:O	1:C:561:ARG:NH2	1.68	1.26
1:A:646:SER:OG	1:A:648:LEU:HD12	1.35	1.21
1:A:647:LYS:HB2	1:A:675:TYR:CE1	1.76	1.20
1:C:527:ASN:HD22	3:F:551:PRO:HB3	1.09	1.10
3:E:254:PRO:C	3:E:256:PRO:HD2	1.74	1.07
3:E:51:ASN:HB3	3:E:53:LYS:HD3	1.35	1.06
3:F:46:LEU:CD2	3:F:85:VAL:HG23	1.90	1.00
3:E:406:CYS:O	3:E:410:THR:HG22	1.62	0.98
3:E:494:LEU:HD12	3:E:495:TRP:N	1.76	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ASN:HD22	3:F:551:PRO:CB	1.76	0.97
1:C:523:LYS:O	1:C:526:THR:HG23	1.64	0.95
3:E:372:MET:O	3:E:381:ARG:HD2	1.64	0.95
1:A:647:LYS:HB2	1:A:675:TYR:CD1	2.02	0.94
1:C:525:LEU:O	1:C:529:GLU:CB	2.15	0.94
1:A:647:LYS:HB2	1:A:675:TYR:HE1	1.30	0.93
3:E:136:LEU:HD21	3:E:139:LYS:HG3	1.52	0.92
3:E:490:ASN:OD1	3:E:495:TRP:CD1	2.23	0.92
3:F:456:LEU:HD13	3:F:459:GLY:HA2	1.49	0.91
3:E:463:ASP:O	3:E:467:ASN:HB2	1.71	0.90
3:F:18:GLU:O	3:F:18:GLU:HG2	1.71	0.90
3:E:494:LEU:CD1	3:E:495:TRP:N	2.35	0.89
3:E:255:PHE:N	3:E:256:PRO:HD2	1.88	0.89
2:D:67:GLU:HG3	2:D:68:CYS:H	1.37	0.87
3:E:255:PHE:CE1	3:E:303:LEU:CD1	2.57	0.87
3:E:52:GLU:O	3:E:55:LYS:HD3	1.74	0.87
1:C:523:LYS:HA	1:C:526:THR:CG2	2.05	0.86
1:C:527:ASN:ND2	3:F:551:PRO:HB3	1.90	0.86
3:F:46:LEU:HD22	3:F:85:VAL:HG23	1.56	0.86
3:E:494:LEU:HD12	3:E:495:TRP:H	1.39	0.86
1:A:487:SER:OG	1:A:491:LYS:NZ	2.08	0.86
1:C:524:HIS:HD2	1:C:569:PHE:HD1	1.24	0.86
3:F:213:PHE:CE2	3:F:282:LEU:HD11	2.11	0.85
1:C:530:PRO:O	1:C:561:ARG:CZ	2.24	0.85
1:C:607:GLN:HG2	1:C:643:LEU:HD21	1.56	0.85
1:A:619:ALA:HB1	1:A:668:LEU:HD11	1.59	0.84
3:F:405:ARG:NH2	3:F:448:SER:OG	2.09	0.84
3:E:490:ASN:OD1	3:E:495:TRP:HD1	1.57	0.84
3:F:279:ASN:C	3:F:279:ASN:ND2	2.30	0.83
3:F:461:GLU:HG2	3:F:515:MET:HE3	1.61	0.83
3:E:255:PHE:CE1	3:E:303:LEU:HD11	2.14	0.83
1:A:626:THR:HG22	1:A:636:LEU:HD23	1.59	0.83
3:E:108:GLU:OE1	3:E:109:LEU:N	2.12	0.83
3:F:279:ASN:C	3:F:279:ASN:HD22	1.83	0.81
3:F:329:GLU:HG3	3:F:380:LEU:HD11	1.62	0.81
3:F:476:ASN:OD1	3:F:479:ARG:NH1	2.13	0.81
3:E:359:LYS:O	3:E:363:THR:HG23	1.80	0.81
3:F:46:LEU:HD21	3:F:85:VAL:HG23	1.62	0.81
1:A:626:THR:HG22	1:A:636:LEU:CD2	2.11	0.81
3:E:154:LEU:HD11	3:E:176:CYS:HB3	1.63	0.80
3:E:362:LEU:O	3:E:365:PRO:HD2	1.82	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:369:VAL:HA	3:F:372:MET:HG2	1.63	0.80
3:F:494:LEU:HB2	3:F:495:TRP:HA	1.64	0.80
1:C:540:LEU:HD22	1:C:545:TRP:CZ2	2.16	0.80
1:C:522:LYS:O	1:C:526:THR:HG22	1.80	0.80
3:E:490:ASN:OD1	3:E:495:TRP:HB2	1.81	0.80
1:C:666:ASP:N	1:C:666:ASP:OD1	2.15	0.79
2:D:45:CYS:SG	2:D:47:ASN:HB2	2.21	0.79
3:E:163:LYS:O	3:E:168:MET:N	2.16	0.79
3:E:170:ASP:N	3:E:170:ASP:OD1	2.15	0.79
3:F:213:PHE:CD2	3:F:282:LEU:CD1	2.66	0.79
1:A:611:LEU:O	2:B:22:PHE:CE2	2.35	0.79
1:C:625:LEU:O	1:C:629:THR:HG22	1.82	0.78
3:F:254:PRO:HB2	3:F:256:PRO:HD2	1.64	0.78
3:E:482:VAL:O	3:E:582:LYS:NZ	2.16	0.78
3:E:487:GLU:HA	3:E:495:TRP:NE1	1.98	0.78
3:E:251:ILE:HG22	3:E:252:GLY:H	1.49	0.77
3:E:255:PHE:N	3:E:256:PRO:CD	2.48	0.77
3:E:520:TYR:HB3	3:E:562:LEU:HD21	1.65	0.77
3:E:456:LEU:HB3	3:E:459:GLY:HA3	1.67	0.76
3:F:326:ARG:HB3	3:F:326:ARG:HH11	1.50	0.76
3:F:213:PHE:HD2	3:F:282:LEU:CD1	1.98	0.76
1:C:563:TYR:OH	3:F:463:ASP:OD2	2.04	0.76
1:C:618:ASP:OD1	1:C:618:ASP:N	2.18	0.76
3:E:456:LEU:HB3	3:E:459:GLY:CA	2.15	0.75
3:E:52:GLU:O	3:E:55:LYS:CD	2.34	0.75
3:E:108:GLU:HG2	3:E:112:GLU:HG3	1.69	0.75
3:E:52:GLU:HB2	3:E:55:LYS:NZ	2.01	0.75
3:F:336:LEU:HD13	3:F:383:LYS:HG2	1.66	0.75
1:A:465:PHE:O	1:A:469:MET:HG2	1.86	0.75
3:F:213:PHE:HE2	3:F:282:LEU:HD11	1.50	0.75
3:E:136:LEU:HD21	3:E:139:LYS:CG	2.17	0.74
3:E:329:GLU:HG3	3:E:377:ILE:HG13	1.69	0.74
1:A:647:LYS:CB	1:A:675:TYR:CD1	2.70	0.74
3:F:291:TYR:CD2	3:F:334:LYS:HE3	2.22	0.74
3:E:105:GLY:O	3:E:108:GLU:HB3	1.87	0.74
3:E:255:PHE:HA	3:E:258:MET:HG3	1.69	0.74
1:C:467:ALA:HB2	1:C:504:LEU:HD11	1.70	0.74
3:E:368:LEU:O	3:E:372:MET:HG3	1.87	0.74
1:C:534:ASP:HB3	2:D:26:LYS:HG2	1.68	0.74
1:A:535:PHE:CE2	1:A:562:SER:HB3	2.23	0.73
3:E:398:GLN:HB2	3:E:440:TRP:CE2	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:487:GLU:HA	3:E:495:TRP:CD1	2.23	0.73
3:F:455:PHE:CE2	3:F:457:PRO:HB3	2.23	0.73
3:F:447:ILE:HD12	3:F:497:GLU:HG3	1.70	0.73
3:E:413:HIS:HD2	3:E:415:GLY:H	1.36	0.73
2:B:46:ARG:HD2	3:E:472:MET:HB3	1.68	0.73
1:C:493:LYS:HZ1	1:C:498:PHE:HD1	1.35	0.73
1:C:428:SER:HA	1:C:431:LYS:HD3	1.70	0.72
3:F:107:LEU:HD12	3:F:149:THR:HG21	1.71	0.72
3:F:54:ASN:O	3:F:58:ILE:HG13	1.90	0.72
2:D:34:ALA:HB1	3:F:373:THR:HG22	1.72	0.72
1:C:528:SER:HB2	3:F:527:SER:O	1.90	0.72
1:C:493:LYS:NZ	1:C:498:PHE:HD1	1.88	0.71
2:B:49:ILE:HG23	2:B:50:MET:HG2	1.71	0.71
3:F:166:ILE:HG13	3:F:168:MET:HG2	1.71	0.71
3:F:218:CYS:HB3	3:F:219:PRO:HD3	1.71	0.71
1:C:593:ASN:OD1	1:C:598:ARG:NH1	2.23	0.71
3:F:13:CYS:HA	3:F:16:LEU:HD12	1.73	0.70
1:C:515:LYS:NZ	1:C:538:GLN:OE1	2.23	0.70
3:E:255:PHE:CE1	3:E:303:LEU:HD13	2.25	0.70
3:E:462:THR:CG2	3:E:467:ASN:ND2	2.53	0.70
3:F:497:GLU:O	3:F:501:ILE:HG12	1.92	0.70
1:C:523:LYS:HA	1:C:526:THR:HG21	1.74	0.70
1:C:593:ASN:ND2	2:D:20:LYS:O	2.24	0.70
3:F:201:ASN:OD1	3:F:201:ASN:N	2.25	0.70
1:A:539:VAL:C	1:A:540:LEU:HD23	2.11	0.70
3:E:258:MET:HB2	3:E:286:MET:HE1	1.74	0.69
3:E:61:MET:O	3:E:64:ASN:ND2	2.25	0.69
1:A:643:LEU:HB3	1:A:649:LEU:HD12	1.75	0.69
3:E:462:THR:HG22	3:E:467:ASN:ND2	2.07	0.69
3:E:50:GLN:O	3:E:51:ASN:HB2	1.91	0.69
1:A:621:THR:HG23	1:A:624:GLN:OE1	1.92	0.69
2:D:79:PHE:HZ	2:D:96:LEU:HD13	1.57	0.69
2:D:52:LEU:H	2:D:52:LEU:HD12	1.57	0.69
3:F:217:LYS:HE3	3:F:281:GLN:OE1	1.93	0.69
1:C:629:THR:HG23	1:C:631:ILE:H	1.56	0.69
3:F:213:PHE:O	3:F:285:SER:OG	2.11	0.69
3:F:401:TYR:OH	3:F:445:GLN:O	2.11	0.69
1:A:539:VAL:O	1:A:540:LEU:HD23	1.93	0.69
2:D:41:ASN:HB2	2:D:47:ASN:O	1.94	0.68
3:F:553:MET:O	3:F:556:LYS:HG2	1.93	0.68
2:D:53:CYS:HB3	2:D:68:CYS:SG	2.33	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:513:LEU:HD13	3:F:569:GLU:HG2	1.74	0.68
1:A:493:LYS:HA	1:A:501:THR:HG21	1.75	0.68
2:D:66:GLU:HG3	2:D:67:GLU:HG2	1.75	0.68
3:F:46:LEU:CD2	3:F:85:VAL:CG2	2.71	0.68
1:C:524:HIS:C	1:C:524:HIS:HD1	1.97	0.68
3:F:362:LEU:O	3:F:366:GLN:HG3	1.93	0.68
1:A:577:ARG:HD3	2:B:33:TRP:CE3	2.28	0.68
1:C:558:GLU:HB3	2:D:24:VAL:HG21	1.75	0.68
3:E:136:LEU:CD2	3:E:139:LYS:HG3	2.24	0.67
1:C:634:ASP:OD1	1:C:634:ASP:N	2.24	0.67
3:F:294:PHE:O	3:F:341:ASN:ND2	2.26	0.67
1:A:614:TYR:HB2	2:B:22:PHE:HE2	1.59	0.67
3:F:14:GLN:HE21	3:F:54:ASN:HD21	1.42	0.67
3:F:161:TYR:HB2	3:F:224:GLN:HE21	1.58	0.67
3:E:57:ILE:O	3:E:61:MET:N	2.28	0.66
3:E:255:PHE:HE1	3:E:303:LEU:CD1	2.06	0.66
3:E:309:PRO:HA	3:E:312:LEU:HD12	1.77	0.66
3:F:148:SER:O	3:F:152:ASN:ND2	2.27	0.66
3:F:385:LEU:HD11	3:F:419:PHE:CE2	2.31	0.66
1:A:646:SER:OG	1:A:648:LEU:CD1	2.30	0.66
1:A:611:LEU:O	2:B:22:PHE:CD2	2.49	0.66
1:C:628:SER:OG	1:C:629:THR:N	2.26	0.66
1:C:476:HIS:O	1:C:478:ASN:ND2	2.29	0.66
1:C:527:ASN:ND2	3:F:551:PRO:CG	2.58	0.66
2:D:67:GLU:HG3	2:D:68:CYS:N	2.09	0.66
3:E:487:GLU:O	3:E:488:ASN:HB2	1.94	0.66
3:E:351:LEU:HB3	3:E:395:LEU:HA	1.78	0.65
1:A:486:ALA:HB2	1:A:508:PHE:CZ	2.32	0.65
1:C:524:HIS:CD2	1:C:569:PHE:HD1	2.11	0.65
3:F:126:LEU:HD13	3:F:183:PHE:HB2	1.77	0.65
3:E:43:ASP:N	3:E:43:ASP:OD1	2.21	0.65
3:F:505:PHE:O	3:F:509:LEU:HB2	1.97	0.65
3:E:486:ASN:O	3:E:495:TRP:NE1	2.27	0.65
1:C:523:LYS:C	1:C:526:THR:HG23	2.17	0.64
1:A:669:ILE:N	1:A:669:ILE:HD12	2.12	0.64
3:E:486:ASN:C	3:E:495:TRP:HE1	2.01	0.64
3:E:255:PHE:HB2	3:E:289:LEU:HD21	1.79	0.64
3:E:255:PHE:CZ	3:E:303:LEU:HD13	2.33	0.64
3:E:567:LEU:O	3:E:570:SER:OG	2.14	0.64
3:E:280:LYS:O	3:E:281:GLN:NE2	2.31	0.64
3:E:255:PHE:HE1	3:E:303:LEU:HD11	1.59	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:280:LYS:H	3:F:280:LYS:HD2	1.62	0.64
3:F:291:TYR:CE2	3:F:334:LYS:HE3	2.33	0.64
3:F:356:LEU:HA	3:F:361:PHE:HB2	1.79	0.64
3:F:480:TYR:CZ	3:F:484:LYS:HG3	2.32	0.64
2:B:94:CYS:HB2	2:B:101:TRP:HE3	1.63	0.64
3:F:352:LEU:HD12	3:F:396:ASP:OD1	1.97	0.63
1:C:493:LYS:NZ	1:C:501:THR:OG1	2.32	0.63
1:C:530:PRO:O	1:C:561:ARG:NH1	2.30	0.63
3:F:46:LEU:O	3:F:50:GLN:CD	2.37	0.63
3:E:462:THR:CG2	3:E:467:ASN:HD22	2.12	0.63
3:E:14:GLN:HB2	3:E:54:ASN:ND2	2.14	0.63
1:C:498:PHE:CZ	1:C:502:SER:HA	2.34	0.63
3:E:416:VAL:O	3:E:420:ILE:HG12	1.98	0.62
3:F:444:PRO:HA	3:F:447:ILE:HG12	1.81	0.62
3:E:490:ASN:ND2	3:E:492:THR:O	2.31	0.62
3:F:181:ILE:HG21	3:F:243:GLU:HG2	1.81	0.62
3:F:439:LYS:HB2	3:F:442:THR:CG2	2.29	0.62
3:E:258:MET:HB2	3:E:286:MET:CE	2.28	0.62
3:E:188:VAL:HG11	3:E:247:PHE:CE1	2.35	0.62
3:E:413:HIS:O	3:E:417:GLU:HG3	1.99	0.62
3:F:203:LYS:O	3:F:207:GLU:HG2	1.99	0.62
3:F:326:ARG:HH11	3:F:326:ARG:CB	2.12	0.61
3:E:218:CYS:HB3	3:E:219:PRO:HD3	1.82	0.61
3:F:431:SER:O	3:F:432:LEU:HD23	2.00	0.61
3:E:67:GLY:O	3:E:71:ARG:HG3	2.00	0.61
3:F:255:PHE:CG	3:F:256:PRO:HD3	2.36	0.61
2:D:55:GLU:O	2:D:59:ASN:ND2	2.34	0.61
3:F:457:PRO:HG2	3:F:458:GLU:HG3	1.82	0.61
3:F:557:VAL:HG23	3:F:558:LEU:HD23	1.82	0.61
2:B:54:ILE:HG23	2:B:55:GLU:N	2.16	0.60
3:E:109:LEU:O	3:E:113:PRO:HD2	2.01	0.60
3:E:136:LEU:HD23	3:E:139:LYS:HB2	1.82	0.60
3:E:369:VAL:HA	3:E:372:MET:SD	2.40	0.60
3:E:46:LEU:HD21	3:E:88:LEU:HD13	1.83	0.60
3:E:487:GLU:CA	3:E:495:TRP:NE1	2.63	0.60
3:F:460:ALA:HB1	3:F:515:MET:CE	2.31	0.60
3:E:487:GLU:N	3:E:495:TRP:CE2	2.70	0.60
1:C:527:ASN:HD22	3:F:551:PRO:CG	2.14	0.60
3:E:286:MET:HE1	3:E:289:LEU:HD23	1.82	0.60
3:E:487:GLU:N	3:E:495:TRP:CZ2	2.69	0.60
1:A:583:TYR:O	1:A:586:SER:N	2.23	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:177:CYS:HB3	3:E:240:PHE:CD1	2.37	0.60
3:E:502:GLU:HA	3:E:506:LEU:HB2	1.82	0.60
2:B:49:ILE:O	2:B:50:MET:HB2	2.01	0.60
1:C:540:LEU:HD13	1:C:545:TRP:CD2	2.37	0.60
3:F:115:GLY:N	3:F:118:ILE:HG13	2.17	0.60
3:F:377:ILE:HG22	3:F:379:THR:HG23	1.83	0.60
1:C:629:THR:OG1	1:C:631:ILE:HG13	2.02	0.60
3:F:105:GLY:O	3:F:108:GLU:HB3	2.02	0.60
3:F:113:PRO:HB2	3:F:117:GLN:HB3	1.82	0.60
1:A:642:ILE:HD11	1:A:688:MET:HA	1.85	0.59
3:E:317:MET:HG3	3:E:361:PHE:CE1	2.38	0.59
3:F:115:GLY:H	3:F:118:ILE:HG13	1.68	0.59
3:F:161:TYR:HB2	3:F:224:GLN:NE2	2.18	0.59
1:A:686:VAL:HG22	1:A:687:PRO:O	2.03	0.59
2:B:53:CYS:HB3	2:B:68:CYS:SG	2.42	0.59
3:F:178:LYS:NZ	3:F:236:PRO:HB3	2.17	0.59
3:F:46:LEU:O	3:F:50:GLN:NE2	2.36	0.58
3:F:46:LEU:HD22	3:F:85:VAL:CG2	2.31	0.58
2:B:90:THR:OG1	2:B:91:ARG:NE	2.37	0.58
3:E:376:PRO:HB2	3:E:377:ILE:HD13	1.84	0.58
3:E:407:LEU:HA	3:E:410:THR:CG2	2.33	0.58
3:E:457:PRO:O	3:E:458:GLU:C	2.39	0.58
3:E:456:LEU:HB3	3:E:459:GLY:HA2	1.85	0.58
1:A:521:PHE:CZ	1:A:525:LEU:HD11	2.38	0.58
1:C:508:PHE:O	1:C:511:ILE:HG12	2.02	0.58
3:E:110:ILE:HG23	3:E:111:GLU:H	1.68	0.58
3:F:17:GLU:O	3:F:18:GLU:HB3	2.04	0.58
3:F:213:PHE:CD2	3:F:282:LEU:HD11	2.35	0.58
1:C:528:SER:HB2	3:F:531:GLN:HG2	1.85	0.58
3:E:362:LEU:C	3:E:365:PRO:HD2	2.24	0.58
3:E:52:GLU:HB2	3:E:55:LYS:HZ3	1.69	0.58
3:F:326:ARG:HH11	3:F:326:ARG:CG	2.16	0.58
1:C:535:PHE:CD1	1:C:536:SER:N	2.72	0.58
3:F:160:PRO:HB2	3:F:166:ILE:HG23	1.86	0.58
3:E:110:ILE:HG23	3:E:111:GLU:N	2.19	0.58
2:B:48:HIS:HB3	2:B:51:ASP:HB2	1.85	0.57
3:F:310:LEU:HD21	3:F:355:TYR:CE1	2.39	0.57
3:E:320:ILE:HD13	3:E:339:LEU:HB2	1.85	0.57
3:E:462:THR:HG21	3:E:467:ASN:ND2	2.18	0.57
1:A:535:PHE:HE2	1:A:562:SER:HB3	1.67	0.57
1:C:528:SER:HB3	3:F:531:GLN:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:133:ILE:HD13	3:E:143:ILE:HG13	1.86	0.57
1:C:474:LEU:HD22	1:C:511:ILE:HD13	1.85	0.57
1:C:523:LYS:CA	1:C:526:THR:CG2	2.79	0.57
3:E:251:ILE:HG22	3:E:252:GLY:N	2.18	0.57
3:F:293:VAL:HG12	3:F:294:PHE:CD1	2.39	0.57
1:C:642:ILE:HD13	1:C:686:VAL:HG23	1.85	0.57
1:C:527:ASN:ND2	3:F:551:PRO:HD3	2.19	0.57
1:C:574:HIS:HB3	1:C:577:ARG:HD3	1.87	0.57
3:E:168:MET:O	3:E:168:MET:HG3	2.04	0.57
1:A:483:ASP:N	1:A:483:ASP:OD2	2.37	0.57
1:A:536:SER:OG	2:B:28:ASN:ND2	2.38	0.57
3:E:100:LYS:O	3:E:104:LEU:HD12	2.04	0.57
3:E:453:VAL:HG23	3:E:454:LEU:HG	1.87	0.57
3:F:279:ASN:O	3:F:279:ASN:ND2	2.38	0.57
3:F:137:HIS:CG	3:F:138:ASN:N	2.73	0.57
3:F:110:ILE:HG23	3:F:153:GLN:NE2	2.19	0.57
3:E:44:GLN:HA	3:E:47:GLU:HB3	1.86	0.57
3:F:495:TRP:N	3:F:495:TRP:CD1	2.73	0.57
1:A:668:LEU:C	1:A:669:ILE:HD12	2.25	0.57
2:D:87:TRP:C	2:D:87:TRP:CD1	2.78	0.57
1:C:484:ALA:HA	1:C:487:SER:HB3	1.87	0.56
3:F:286:MET:HB3	3:F:319:HIS:HE1	1.70	0.56
3:F:351:LEU:O	3:F:396:ASP:N	2.38	0.56
3:F:356:LEU:HA	3:F:361:PHE:CB	2.34	0.56
2:B:94:CYS:HB2	2:B:101:TRP:CE3	2.40	0.56
3:E:494:LEU:HD13	3:E:495:TRP:N	2.18	0.56
1:C:528:SER:CB	3:F:531:GLN:HG2	2.34	0.56
2:D:66:GLU:HG3	2:D:67:GLU:H	1.70	0.56
1:C:503:LYS:HD2	1:C:544:SER:HA	1.87	0.56
3:E:254:PRO:HB2	3:E:256:PRO:HD2	1.87	0.56
3:E:490:ASN:CG	3:E:495:TRP:HD1	2.08	0.56
1:C:510:ASP:O	1:C:514:SER:OG	2.22	0.56
2:D:77:HIS:CE1	2:D:97:ASP:OD1	2.58	0.56
1:C:507:MET:HG2	1:C:545:TRP:CE2	2.40	0.56
3:E:487:GLU:CA	3:E:495:TRP:CE2	2.88	0.56
3:F:279:ASN:HD22	3:F:280:LYS:N	2.02	0.56
3:F:392:ILE:O	3:F:400:LYS:NZ	2.38	0.56
1:C:621:THR:HG23	1:C:624:GLN:OE1	2.06	0.56
3:E:353:TYR:N	3:E:396:ASP:OD2	2.39	0.56
3:F:367:GLY:O	3:F:371:VAL:HG23	2.05	0.56
1:A:532:ASP:OD1	1:A:532:ASP:N	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:SER:OG	3:E:527:SER:OG	2.14	0.55
1:A:444:ASP:OD2	1:A:448:GLN:NE2	2.40	0.55
1:C:661:VAL:HG13	1:C:662:GLU:N	2.20	0.55
3:F:531:GLN:O	3:F:532:LYS:HE3	2.06	0.55
3:E:377:ILE:N	3:E:377:ILE:HD13	2.22	0.55
3:F:5:GLU:OE1	3:F:35:ARG:NH1	2.38	0.55
3:E:51:ASN:O	3:E:52:GLU:HG2	2.05	0.55
3:F:180:LEU:O	3:F:184:THR:OG1	2.23	0.55
1:A:597:ASN:HD22	1:C:657:ASN:HD21	1.55	0.55
3:E:107:LEU:O	3:E:110:ILE:HG22	2.07	0.55
2:D:46:ARG:O	3:F:422:GLN:NE2	2.40	0.55
3:E:490:ASN:OD1	3:E:495:TRP:CB	2.54	0.55
3:E:80:ASP:H	3:E:83:ARG:HE	1.55	0.55
3:F:256:PRO:O	3:F:257:LYS:HB2	2.07	0.55
3:F:320:ILE:CD1	3:F:339:LEU:HA	2.37	0.55
3:F:485:ASP:OD2	3:F:492:THR:OG1	2.23	0.55
3:F:140:ALA:HA	3:F:143:ILE:HD12	1.88	0.54
1:A:582:LEU:HD11	2:B:32:LEU:HG	1.90	0.54
1:A:612:LEU:HD23	2:B:22:PHE:CB	2.37	0.54
3:F:528:GLN:O	3:F:531:GLN:HG3	2.07	0.54
1:C:589:GLU:OE1	2:D:26:LYS:HD3	2.07	0.54
3:E:181:ILE:HG21	3:E:243:GLU:HG2	1.90	0.54
3:E:510:HIS:NE2	3:E:576:GLU:OE1	2.24	0.54
3:F:181:ILE:HD11	3:F:240:PHE:CD1	2.42	0.54
1:A:607:GLN:HG2	1:A:643:LEU:HD21	1.90	0.54
1:C:488:MET:O	1:C:492:LEU:HB2	2.07	0.54
1:C:444:ASP:O	1:C:447:ASN:ND2	2.41	0.54
1:C:540:LEU:HB3	1:C:545:TRP:CD1	2.41	0.54
3:F:151:TRP:NE1	3:F:214:LYS:HB3	2.22	0.54
2:D:93:VAL:HG22	2:D:94:CYS:H	1.73	0.54
3:E:406:CYS:C	3:E:410:THR:HG22	2.28	0.54
3:F:427:GLN:O	3:F:431:SER:OG	2.21	0.54
1:C:558:GLU:N	1:C:558:GLU:OE1	2.40	0.54
3:E:45:LEU:HD22	3:E:89:ILE:HD11	1.90	0.54
2:D:47:ASN:ND2	2:D:54:ILE:HA	2.22	0.53
3:E:405:ARG:NH2	3:E:448:SER:OG	2.41	0.53
3:E:417:GLU:O	3:E:421:ILE:HG13	2.08	0.53
3:F:247:PHE:O	3:F:251:ILE:HD13	2.08	0.53
1:A:647:LYS:NZ	1:A:676:LYS:O	2.22	0.53
2:B:53:CYS:HA	2:B:80:HIS:CE1	2.43	0.53
2:D:79:PHE:CZ	2:D:96:LEU:HD13	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:GLN:HB2	1:A:683:ASN:HA	1.90	0.53
1:C:527:ASN:ND2	3:F:551:PRO:CD	2.72	0.53
1:C:664:LYS:HB2	1:C:667:THR:HG23	1.90	0.53
1:A:429:LEU:HG	1:A:430:LEU:N	2.22	0.53
2:B:94:CYS:SG	2:B:95:PRO:HD2	2.48	0.53
3:E:160:PRO:O	3:E:161:TYR:CD1	2.62	0.53
3:F:242:SER:HB2	3:F:298:ILE:HD13	1.91	0.53
3:F:99:PRO:O	3:F:103:LEU:HB2	2.09	0.53
1:A:427:ASP:HB2	1:A:473:ARG:HE	1.74	0.53
3:F:406:CYS:O	3:F:410:THR:OG1	2.26	0.53
1:A:535:PHE:CD2	1:A:562:SER:HB3	2.44	0.53
2:B:62:SER:H	2:B:65:SER:HB2	1.74	0.53
3:E:326:ARG:NH1	3:E:328:GLU:OE2	2.41	0.53
3:E:413:HIS:CD2	3:E:415:GLY:H	2.22	0.53
3:F:6:LEU:HB2	3:F:32:ALA:HB1	1.90	0.53
3:F:507:LYS:N	3:F:508:PRO:HD2	2.24	0.53
1:C:507:MET:HG2	1:C:545:TRP:CD2	2.44	0.53
3:F:170:ASP:N	3:F:170:ASP:OD2	2.42	0.53
2:D:94:CYS:HB3	2:D:97:ASP:HB2	1.90	0.52
3:F:104:LEU:HA	3:F:107:LEU:HB2	1.90	0.52
1:A:621:THR:OG1	1:A:624:GLN:HG3	2.09	0.52
2:D:36:ASP:OD1	2:D:37:ILE:N	2.42	0.52
3:E:92:LEU:O	3:E:96:LEU:HG	2.09	0.52
3:F:74:LEU:HD21	3:F:124:LEU:HD22	1.92	0.52
3:F:47:GLU:O	3:F:50:GLN:HG2	2.10	0.52
3:E:199:LEU:HD12	3:E:202:GLU:HB2	1.90	0.52
3:E:499:GLY:O	3:E:502:GLU:HG2	2.09	0.52
3:E:576:GLU:HA	3:E:579:ILE:HB	1.92	0.52
3:F:303:LEU:HG	3:F:304:PRO:HD2	1.92	0.52
3:F:439:LYS:HB2	3:F:442:THR:HG21	1.91	0.52
3:F:154:LEU:HD12	3:F:155:SER:N	2.25	0.52
3:F:375:CYS:O	3:F:381:ARG:HD3	2.09	0.52
1:A:426:CYS:O	1:A:430:LEU:HB2	2.10	0.52
3:F:121:SER:O	3:F:125:LEU:HB2	2.08	0.52
3:F:255:PHE:CD2	3:F:256:PRO:HD3	2.45	0.52
3:F:213:PHE:HD2	3:F:282:LEU:HD12	1.73	0.52
3:F:328:GLU:N	3:F:328:GLU:OE2	2.32	0.52
3:F:72:CYS:HG	3:F:86:TYR:HE2	1.55	0.52
1:A:426:CYS:HA	1:A:429:LEU:HD23	1.91	0.52
3:E:300:ILE:HG12	3:E:300:ILE:O	2.10	0.52
3:F:293:VAL:O	3:F:300:ILE:HD11	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:447:ILE:HD11	3:F:493:GLY:HA2	1.92	0.52
3:E:346:ILE:HG22	3:E:347:GLU:O	2.09	0.51
3:E:490:ASN:OD1	3:E:495:TRP:CG	2.63	0.51
3:F:443:GLY:O	3:F:446:LEU:N	2.29	0.51
3:F:479:ARG:O	3:F:483:ILE:HG13	2.10	0.51
2:B:58:ALA:HB2	3:E:480:TYR:CD1	2.45	0.51
1:A:537:ILE:HG21	1:A:566:PHE:CZ	2.45	0.51
1:A:671:LEU:HD12	1:A:672:TYR:N	2.25	0.51
3:E:258:MET:CB	3:E:286:MET:CE	2.88	0.51
3:F:255:PHE:O	3:F:258:MET:HB2	2.09	0.51
3:F:460:ALA:HB1	3:F:515:MET:HE1	1.93	0.51
1:A:647:LYS:CB	1:A:675:TYR:HD1	2.23	0.51
3:E:195:LYS:HG2	3:E:196:GLU:N	2.26	0.51
3:E:413:HIS:HB3	3:E:416:VAL:HG13	1.91	0.51
3:E:66:VAL:HG23	3:E:93:LEU:HD13	1.91	0.51
2:B:40:ASP:HB2	2:B:48:HIS:CE1	2.46	0.51
1:C:493:LYS:NZ	1:C:498:PHE:CD1	2.75	0.51
1:C:540:LEU:HD22	1:C:545:TRP:CE2	2.45	0.51
1:C:559:LEU:HD13	2:D:27:TRP:CE2	2.45	0.51
3:E:486:ASN:C	3:E:495:TRP:NE1	2.63	0.51
1:C:524:HIS:ND1	1:C:524:HIS:C	2.58	0.51
3:E:494:LEU:C	3:E:494:LEU:CD1	2.77	0.51
3:F:329:GLU:HG3	3:F:380:LEU:CD1	2.37	0.51
3:F:388:LEU:O	3:F:392:ILE:HG13	2.11	0.51
3:F:460:ALA:HB1	3:F:515:MET:HE2	1.93	0.51
1:C:481:SER:OG	1:C:484:ALA:N	2.43	0.50
1:C:527:ASN:ND2	3:F:551:PRO:CB	2.55	0.50
2:D:72:TRP:CD2	2:D:78:ALA:HB2	2.46	0.50
3:E:450:LEU:HA	3:E:453:VAL:HG22	1.94	0.50
3:F:95:LYS:O	3:F:135:LYS:NZ	2.42	0.50
3:E:494:LEU:O	3:E:497:GLU:N	2.45	0.50
3:F:30:GLN:HG3	3:F:64:ASN:HB3	1.94	0.50
3:E:507:LYS:N	3:E:508:PRO:HD2	2.27	0.50
3:F:129:LEU:O	3:F:133:ILE:HG13	2.12	0.50
3:F:220:LEU:HD13	3:F:292:LEU:HD11	1.94	0.50
3:E:238:ARG:HG3	3:E:298:ILE:HD11	1.93	0.50
3:E:413:HIS:HD2	3:E:415:GLY:N	2.06	0.50
3:E:424:ILE:O	3:E:428:ILE:HG13	2.11	0.50
3:F:323:PHE:HD1	3:F:331:VAL:HG12	1.76	0.50
3:E:10:ILE:HD11	3:E:29:PHE:HE1	1.77	0.49
3:E:177:CYS:O	3:E:181:ILE:HG12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:THR:CG2	1:A:636:LEU:HD23	2.36	0.49
3:E:90:PHE:O	3:E:94:VAL:HG13	2.12	0.49
3:F:17:GLU:O	3:F:18:GLU:OE2	2.30	0.49
3:F:299:HIS:HB3	3:F:302:GLN:HG3	1.94	0.49
3:F:352:LEU:O	3:F:355:TYR:HD2	1.95	0.49
1:C:527:ASN:O	1:C:529:GLU:HG2	2.12	0.49
3:E:577:GLU:O	3:E:581:ILE:HD13	2.12	0.49
3:F:130:GLN:OE1	3:F:183:PHE:HA	2.12	0.49
3:F:424:ILE:O	3:F:428:ILE:HG13	2.13	0.49
3:F:63:TRP:O	3:F:66:VAL:HG12	2.11	0.49
2:B:58:ALA:HB2	3:E:480:TYR:HD1	1.78	0.49
2:B:62:SER:H	2:B:65:SER:CB	2.25	0.49
3:F:478:LEU:HD12	3:F:575:VAL:HG11	1.94	0.49
1:C:540:LEU:O	2:D:32:LEU:HA	2.13	0.49
2:B:88:LEU:HD11	2:B:101:TRP:CD1	2.48	0.49
1:C:623:GLN:O	1:C:626:THR:HG22	2.13	0.49
3:E:375:CYS:HA	3:E:376:PRO:HD3	1.72	0.49
1:A:582:LEU:HB3	1:A:584:GLN:NE2	2.28	0.49
1:C:524:HIS:HD2	1:C:569:PHE:CD1	2.16	0.49
3:E:520:TYR:CB	3:E:562:LEU:HD21	2.38	0.49
3:F:339:LEU:O	3:F:342:SER:HB2	2.13	0.49
1:C:471:ALA:O	1:C:475:VAL:HG12	2.12	0.49
3:E:118:ILE:HG22	3:E:119:SER:N	2.28	0.49
3:F:73:LEU:HD22	3:F:87:PHE:CE2	2.47	0.49
2:B:87:TRP:CE2	2:B:95:PRO:HB3	2.49	0.48
2:D:47:ASN:HD22	2:D:54:ILE:HA	1.77	0.48
3:F:249:SER:HB3	3:F:302:GLN:HE22	1.78	0.48
3:F:143:ILE:HD13	3:F:204:LEU:HD13	1.93	0.48
3:F:351:LEU:HB3	3:F:395:LEU:HA	1.94	0.48
1:A:662:GLU:O	1:A:662:GLU:HG2	2.13	0.48
1:A:612:LEU:HD23	2:B:22:PHE:HB3	1.95	0.48
1:C:527:ASN:ND2	3:F:551:PRO:HG3	2.27	0.48
3:F:66:VAL:HG21	3:F:106:LEU:HD23	1.95	0.48
3:F:107:LEU:O	3:F:110:ILE:HG13	2.13	0.48
3:F:466:GLN:HE21	3:F:466:GLN:HA	1.79	0.48
3:F:512:GLY:O	3:F:516:SER:OG	2.31	0.48
3:E:365:PRO:O	3:E:368:LEU:HB2	2.13	0.48
3:F:414:SER:OG	3:F:467:ASN:HA	2.13	0.48
1:A:521:PHE:CE2	1:A:525:LEU:HD11	2.49	0.48
3:E:532:LYS:HG2	3:E:533:SER:N	2.28	0.48
3:E:53:LYS:HA	3:E:54:ASN:HA	1.58	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:106:LEU:HD22	3:E:125:LEU:HD23	1.94	0.48
3:E:254:PRO:CB	3:E:256:PRO:HD2	2.43	0.48
3:E:487:GLU:HA	3:E:495:TRP:CE2	2.48	0.48
2:D:25:LYS:HG2	2:D:26:LYS:HG3	1.96	0.48
3:E:254:PRO:HB2	3:E:256:PRO:CD	2.44	0.48
3:F:178:LYS:HZ3	3:F:236:PRO:HB3	1.79	0.48
1:A:616:THR:OG1	1:A:620:TYR:OH	2.26	0.48
3:E:52:GLU:HB2	3:E:55:LYS:HZ2	1.79	0.48
3:E:45:LEU:HD22	3:E:89:ILE:CD1	2.44	0.48
1:A:553:PHE:CD1	1:A:606:PHE:HE1	2.31	0.47
1:A:611:LEU:O	2:B:22:PHE:HE2	1.93	0.47
1:A:572:SER:OG	3:E:557:VAL:HB	2.14	0.47
1:A:470:LEU:HG	1:A:474:LEU:HD22	1.95	0.47
2:B:49:ILE:O	2:B:50:MET:CB	2.60	0.47
3:E:414:SER:HB2	3:E:469:ASP:OD1	2.14	0.47
3:E:487:GLU:N	3:E:495:TRP:NE1	2.62	0.47
3:F:450:LEU:O	3:F:453:VAL:N	2.46	0.47
1:A:556:PRO:O	1:A:559:LEU:N	2.42	0.47
1:C:545:TRP:HA	1:C:546:PRO:HD3	1.68	0.47
3:F:34:GLN:HE21	3:F:34:GLN:HB3	1.56	0.47
3:F:398:GLN:HB2	3:F:440:TRP:CE2	2.49	0.47
3:F:550:PRO:O	3:F:553:MET:HB2	2.15	0.47
1:A:482:ASP:N	1:A:482:ASP:OD1	2.47	0.47
3:F:362:LEU:C	3:F:365:PRO:HD2	2.35	0.47
1:C:540:LEU:HB3	1:C:545:TRP:NE1	2.29	0.47
3:E:328:GLU:O	3:E:332:ILE:HD12	2.13	0.47
3:E:550:PRO:HG2	3:E:551:PRO:HD3	1.97	0.47
1:A:524:HIS:HD2	3:E:554:GLN:OE1	1.97	0.47
1:A:540:LEU:HD13	1:A:545:TRP:CD2	2.49	0.47
3:F:242:SER:HA	3:F:298:ILE:HG21	1.97	0.47
3:F:9:ILE:HG23	3:F:25:ASP:OD1	2.15	0.47
1:C:501:THR:HA	1:C:504:LEU:HD23	1.97	0.47
1:C:673:LEU:HD12	1:C:673:LEU:N	2.30	0.47
2:D:72:TRP:CE3	2:D:78:ALA:HB2	2.48	0.47
3:F:300:ILE:O	3:F:300:ILE:HG22	2.15	0.47
3:E:238:ARG:NH2	3:E:296:GLN:O	2.47	0.47
3:F:109:LEU:HD12	3:F:110:ILE:N	2.29	0.47
1:A:559:LEU:HD22	2:B:27:TRP:CE3	2.50	0.47
2:D:96:LEU:N	2:D:96:LEU:HD12	2.30	0.47
3:E:258:MET:CB	3:E:286:MET:HE1	2.42	0.47
3:E:41:HIS:H	3:E:41:HIS:CD2	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:494:LEU:HD11	3:E:495:TRP:CD2	2.50	0.47
3:E:500:ASN:N	3:E:500:ASN:OD1	2.45	0.47
3:F:177:CYS:HB3	3:F:240:PHE:CE1	2.50	0.47
3:F:85:VAL:HG13	3:F:86:TYR:HD1	1.79	0.47
1:A:613:GLN:O	1:A:620:TYR:HE2	1.98	0.47
3:E:326:ARG:CG	3:E:326:ARG:HH11	2.28	0.47
3:F:326:ARG:NH1	3:F:326:ARG:CG	2.78	0.47
1:A:493:LYS:HA	1:A:501:THR:CG2	2.45	0.47
1:A:675:TYR:OH	1:A:677:ASN:ND2	2.47	0.47
3:F:27:GLY:O	3:F:31:LEU:HB2	2.15	0.47
2:B:54:ILE:CG2	2:B:55:GLU:N	2.77	0.46
2:D:67:GLU:CG	2:D:68:CYS:H	2.17	0.46
3:E:462:THR:HG22	3:E:467:ASN:HD22	1.75	0.46
1:A:534:ASP:HB3	2:B:26:LYS:HG2	1.97	0.46
3:E:365:PRO:HA	3:E:368:LEU:HD12	1.95	0.46
3:E:461:GLU:HG2	3:E:461:GLU:H	1.57	0.46
3:F:17:GLU:O	3:F:18:GLU:CB	2.63	0.46
3:F:151:TRP:CD1	3:F:214:LYS:HB3	2.50	0.46
3:F:320:ILE:HD11	3:F:339:LEU:HA	1.97	0.46
3:F:466:GLN:O	3:F:467:ASN:HB2	2.16	0.46
1:A:668:LEU:HD12	1:A:669:ILE:N	2.30	0.46
1:C:521:PHE:O	1:C:524:HIS:HB3	2.15	0.46
3:E:398:GLN:HB2	3:E:440:TRP:CD2	2.51	0.46
3:F:218:CYS:CB	3:F:219:PRO:HD3	2.40	0.46
3:F:404:PHE:CD2	3:F:424:ILE:HG12	2.50	0.46
1:A:689:LYS:HE2	1:A:689:LYS:H	1.80	0.46
3:E:127:GLN:HB3	3:E:128:PRO:HD3	1.96	0.46
3:E:443:GLY:O	3:E:446:LEU:N	2.48	0.46
3:F:575:VAL:O	3:F:579:ILE:HG13	2.16	0.46
1:A:471:ALA:O	1:A:475:VAL:HG22	2.15	0.46
2:D:75:CYS:HB2	2:D:97:ASP:OD2	2.14	0.46
3:E:188:VAL:HG11	3:E:247:PHE:CD1	2.50	0.46
3:E:353:TYR:HB2	3:E:398:GLN:HG2	1.98	0.46
1:A:420:GLU:OE2	1:A:424:ARG:NH1	2.49	0.46
1:A:614:TYR:CE1	1:A:649:LEU:HD21	2.51	0.46
1:A:626:THR:HG22	1:A:636:LEU:HD22	1.96	0.46
3:E:336:LEU:HD13	3:E:383:LYS:HG2	1.98	0.46
3:E:407:LEU:HA	3:E:410:THR:HG23	1.97	0.46
3:E:91:ASP:O	3:E:94:VAL:HG22	2.14	0.46
3:F:582:LYS:HB3	3:F:582:LYS:HE2	1.47	0.46
1:A:669:ILE:CD1	1:A:669:ILE:N	2.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:125:LEU:N	3:E:125:LEU:HD12	2.31	0.46
3:E:320:ILE:HD13	3:E:339:LEU:CA	2.46	0.46
3:F:122:ILE:HG22	3:F:126:LEU:HD23	1.98	0.46
3:F:211:PHE:O	3:F:215:SER:OG	2.34	0.46
3:F:45:LEU:O	3:F:46:LEU:CB	2.64	0.46
3:E:425:LYS:HE2	3:E:425:LYS:HB3	1.62	0.46
3:E:509:LEU:HD23	3:E:572:LEU:HD22	1.98	0.46
3:F:112:GLU:O	3:F:113:PRO:O	2.33	0.46
3:F:115:GLY:H	3:F:118:ILE:H	1.62	0.46
1:A:641:GLN:HE21	1:A:641:GLN:HB3	1.42	0.46
1:A:688:MET:HB2	1:A:688:MET:HE3	1.77	0.46
3:F:130:GLN:O	3:F:134:GLN:HG2	2.16	0.46
1:A:527:ASN:O	3:E:531:GLN:HG3	2.16	0.46
3:F:166:ILE:O	3:F:166:ILE:HG12	2.13	0.46
2:B:42:CYS:O	2:B:45:CYS:O	2.34	0.45
3:E:125:LEU:C	3:E:128:PRO:HD2	2.36	0.45
3:E:133:ILE:O	3:E:136:LEU:O	2.34	0.45
3:E:255:PHE:CZ	3:E:303:LEU:CD1	2.94	0.45
3:E:320:ILE:HD13	3:E:339:LEU:CB	2.46	0.45
1:A:508:PHE:O	1:A:511:ILE:N	2.49	0.45
1:A:621:THR:HG23	1:A:624:GLN:CD	2.37	0.45
1:C:621:THR:HG23	1:C:624:GLN:CD	2.37	0.45
2:B:45:CYS:HB2	3:E:476:ASN:OD1	2.17	0.45
1:C:516:ASP:O	1:C:520:GLN:HG2	2.16	0.45
3:E:13:CYS:O	3:E:16:LEU:HG	2.17	0.45
3:F:45:LEU:O	3:F:46:LEU:HB2	2.16	0.45
1:A:565:ARG:HA	1:A:565:ARG:HD2	1.68	0.45
1:C:498:PHE:CE2	1:C:502:SER:HA	2.52	0.45
1:C:524:HIS:CD2	1:C:569:PHE:CD1	3.00	0.45
3:E:434:ARG:NH1	3:E:434:ARG:HB2	2.31	0.45
3:E:83:ARG:HD2	3:E:87:PHE:HE1	1.82	0.45
3:F:281:GLN:HA	3:F:281:GLN:OE1	2.16	0.45
2:B:48:HIS:ND1	2:B:49:ILE:O	2.49	0.45
1:C:492:LEU:C	1:C:492:LEU:HD13	2.37	0.45
3:E:286:MET:CE	3:E:289:LEU:HD23	2.45	0.45
3:E:220:LEU:O	3:E:334:LYS:NZ	2.49	0.45
3:F:465:LEU:HD11	3:F:561:ALA:HB1	1.98	0.45
3:F:92:LEU:HD23	3:F:95:LYS:HD3	1.98	0.45
1:A:612:LEU:HD23	2:B:22:PHE:HB2	1.97	0.45
1:A:689:LYS:N	1:A:689:LYS:HE2	2.32	0.45
3:F:213:PHE:CD2	3:F:282:LEU:HD12	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:180:LEU:HD13	3:E:211:PHE:CZ	2.52	0.45
3:F:151:TRP:CE2	3:F:214:LYS:HB3	2.51	0.45
3:F:326:ARG:NH1	3:F:328:GLU:OE2	2.49	0.45
3:F:447:ILE:CD1	3:F:493:GLY:HA2	2.46	0.45
3:E:235:ASP:O	3:E:238:ARG:N	2.45	0.45
1:A:535:PHE:CD1	1:A:535:PHE:C	2.89	0.45
3:E:106:LEU:O	3:E:109:LEU:HD23	2.17	0.45
3:E:465:LEU:HA	3:E:465:LEU:HD22	1.61	0.45
3:E:52:GLU:HB2	3:E:55:LYS:HD3	1.99	0.45
3:E:582:LYS:HB3	3:E:582:LYS:HE2	1.86	0.45
3:E:6:LEU:O	3:E:6:LEU:HD12	2.17	0.45
3:E:218:CYS:CB	3:E:219:PRO:HD3	2.46	0.45
3:E:359:LYS:HB3	3:E:359:LYS:HE2	1.63	0.45
3:F:116:LYS:HB3	3:F:116:LYS:NZ	2.32	0.45
3:F:385:LEU:O	3:F:385:LEU:HD12	2.16	0.45
1:A:523:LYS:HA	1:A:523:LYS:HD2	1.73	0.44
1:A:537:ILE:HG13	2:B:29:ALA:O	2.17	0.44
1:C:470:LEU:HD22	1:C:507:MET:HE2	1.99	0.44
1:C:645:LYS:HD2	1:C:645:LYS:HA	1.82	0.44
2:D:90:THR:OG1	2:D:91:ARG:NH1	2.50	0.44
3:E:343:LEU:HA	3:E:343:LEU:HD23	1.79	0.44
3:E:352:LEU:HA	3:E:396:ASP:OD2	2.18	0.44
3:E:494:LEU:CD1	3:E:495:TRP:CD2	3.00	0.44
3:F:354:GLN:O	3:F:357:GLU:HB2	2.16	0.44
2:D:37:ILE:HD12	2:D:37:ILE:HA	1.59	0.44
2:D:97:ASP:CB	2:D:99:ARG:H	2.30	0.44
3:E:148:SER:OG	3:E:214:LYS:NZ	2.51	0.44
3:E:95:LYS:O	3:E:135:LYS:NZ	2.50	0.44
3:F:166:ILE:HD11	3:F:170:ASP:H	1.81	0.44
3:F:417:GLU:O	3:F:421:ILE:HG13	2.17	0.44
3:F:93:LEU:O	3:F:97:CYS:HB2	2.17	0.44
3:E:212:CYS:O	3:E:216:LEU:HB2	2.16	0.44
3:F:10:ILE:O	3:F:14:GLN:HG3	2.18	0.44
3:F:320:ILE:HD13	3:F:339:LEU:HB2	2.00	0.44
3:F:456:LEU:HB3	3:F:459:GLY:H	1.81	0.44
3:F:56:VAL:O	3:F:59:LYS:HG3	2.16	0.44
2:B:75:CYS:O	2:B:76:ASN:HB2	2.18	0.44
3:E:217:LYS:O	3:E:221:LEU:HB2	2.17	0.44
3:E:44:GLN:HG2	3:E:44:GLN:H	1.48	0.44
3:F:320:ILE:HD13	3:F:339:LEU:HA	1.99	0.44
3:F:356:LEU:HD13	3:F:402:THR:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:439:LYS:HE2	3:F:442:THR:HG21	1.99	0.44
1:A:506:ARG:O	1:A:510:ASP:HB2	2.17	0.44
3:E:103:LEU:O	3:E:107:LEU:N	2.38	0.44
3:F:185:LYS:N	3:F:186:PRO:HD2	2.33	0.44
3:F:421:ILE:O	3:F:424:ILE:HB	2.17	0.44
3:F:514:ASN:OD1	3:F:514:ASN:N	2.51	0.44
1:A:597:ASN:HD22	1:C:657:ASN:ND2	2.13	0.44
1:A:553:PHE:CD1	1:A:606:PHE:CE1	3.06	0.44
2:B:49:ILE:HD12	2:B:49:ILE:HA	1.89	0.44
2:D:93:VAL:HG23	2:D:100:GLU:HA	1.98	0.44
3:E:57:ILE:HG22	3:E:61:MET:HB2	1.99	0.44
3:E:82:LYS:O	3:E:85:VAL:HG22	2.18	0.44
3:F:364:VAL:N	3:F:365:PRO:CD	2.81	0.44
1:C:527:ASN:HD21	3:F:551:PRO:HD3	1.83	0.44
2:B:35:TRP:O	3:E:413:HIS:HE1	2.01	0.44
1:A:478:ASN:OD1	1:A:479:SER:N	2.49	0.44
1:C:559:LEU:HD13	2:D:27:TRP:CD2	2.53	0.44
3:E:110:ILE:CG2	3:E:111:GLU:H	2.31	0.44
3:E:486:ASN:N	3:E:486:ASN:OD1	2.51	0.44
3:F:574:ARG:NH2	3:F:578:LEU:HD21	2.33	0.44
3:F:49:ILE:HG23	3:F:58:ILE:HD13	1.99	0.44
3:F:72:CYS:SG	3:F:86:TYR:CE2	3.11	0.44
3:E:76:LYS:HD2	3:E:76:LYS:HA	1.78	0.43
1:A:535:PHE:HE1	1:A:537:ILE:HB	1.83	0.43
1:C:623:GLN:NE2	1:C:627:ASP:OD1	2.51	0.43
3:F:140:ALA:HB2	3:F:204:LEU:HB2	2.00	0.43
3:F:465:LEU:HD13	3:F:565:PHE:CZ	2.52	0.43
1:C:661:VAL:HG22	1:C:662:GLU:H	1.83	0.43
3:E:103:LEU:HA	3:E:106:LEU:HD12	1.99	0.43
3:E:450:LEU:HD12	3:E:450:LEU:HA	1.78	0.43
3:E:66:VAL:CG2	3:E:93:LEU:HD13	2.49	0.43
1:C:528:SER:HB3	3:F:531:GLN:CG	2.49	0.43
3:E:291:TYR:CD2	3:E:334:LYS:HE3	2.54	0.43
3:F:383:LYS:O	3:F:386:ALA:HB3	2.18	0.43
1:A:643:LEU:CB	1:A:649:LEU:HD12	2.45	0.43
3:E:188:VAL:O	3:E:192:ILE:HG13	2.17	0.43
3:E:525:LYS:HB3	3:E:525:LYS:HE3	1.89	0.43
1:C:659:ASP:OD1	1:C:659:ASP:N	2.51	0.43
1:C:558:GLU:CB	2:D:24:VAL:HG21	2.46	0.43
3:E:92:LEU:HD12	3:E:92:LEU:O	2.18	0.43
3:F:390:LEU:HA	3:F:390:LEU:HD12	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:130:GLN:HG3	3:F:187:PHE:CZ	2.54	0.43
3:F:563:PHE:O	3:F:566:ASP:HB2	2.18	0.43
1:A:535:PHE:CD1	1:A:536:SER:N	2.86	0.43
1:A:549:GLN:O	1:A:550:SER:OG	2.34	0.43
1:A:559:LEU:HD13	2:B:27:TRP:CE2	2.54	0.43
3:E:363:THR:O	3:E:366:GLN:HB2	2.18	0.43
3:E:398:GLN:HB2	3:E:440:TRP:CZ2	2.54	0.43
1:A:474:LEU:HD12	1:A:474:LEU:HA	1.74	0.43
1:A:561:ARG:O	1:A:562:SER:C	2.56	0.43
3:F:351:LEU:HD12	3:F:351:LEU:HA	1.67	0.43
1:A:671:LEU:HD12	1:A:672:TYR:H	1.82	0.43
3:E:129:LEU:HD23	3:E:129:LEU:HA	1.68	0.43
1:A:422:LEU:HG	1:A:422:LEU:H	1.54	0.42
1:C:430:LEU:HD23	1:C:473:ARG:NH1	2.34	0.42
2:D:93:VAL:HG21	2:D:98:ASN:OD1	2.19	0.42
3:E:180:LEU:O	3:E:184:THR:OG1	2.36	0.42
3:E:59:LYS:HA	3:E:96:LEU:O	2.18	0.42
3:F:458:GLU:HB2	3:F:462:THR:HA	2.00	0.42
3:F:74:LEU:HD22	3:F:120:GLN:HG2	2.01	0.42
1:A:428:SER:HA	1:A:431:LYS:HE3	2.00	0.42
1:A:501:THR:O	1:A:504:LEU:N	2.49	0.42
1:A:540:LEU:HD13	1:A:545:TRP:CE3	2.54	0.42
2:B:87:TRP:CE2	2:B:91:ARG:HG3	2.54	0.42
3:E:138:ASN:O	3:E:200:GLU:HG2	2.19	0.42
3:E:306:VAL:HB	3:E:307:LEU:H	1.46	0.42
3:E:343:LEU:HD22	3:E:394:LYS:HG3	2.00	0.42
3:E:552:GLU:OE1	3:E:552:GLU:O	2.37	0.42
3:F:125:LEU:O	3:F:128:PRO:HG2	2.19	0.42
3:F:302:GLN:HE21	3:F:302:GLN:HB3	1.62	0.42
3:F:66:VAL:HG21	3:F:106:LEU:CD2	2.49	0.42
1:A:614:TYR:HB2	2:B:22:PHE:CE2	2.48	0.42
1:C:482:ASP:O	1:C:485:GLU:HB2	2.18	0.42
3:E:551:PRO:O	3:E:552:GLU:HB3	2.19	0.42
3:F:326:ARG:HH12	3:F:328:GLU:CD	2.23	0.42
3:F:499:GLY:O	3:F:503:ASN:ND2	2.52	0.42
1:A:559:LEU:HD13	2:B:27:TRP:CZ2	2.54	0.42
1:C:467:ALA:HB2	1:C:504:LEU:CD1	2.47	0.42
1:C:478:ASN:HD22	1:C:478:ASN:N	2.17	0.42
3:E:417:GLU:OE1	3:E:470:ARG:HD2	2.19	0.42
3:F:375:CYS:SG	3:F:376:PRO:HD2	2.59	0.42
3:F:329:GLU:CD	3:F:377:ILE:HD12	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:72:CYS:SG	3:F:86:TYR:HE2	2.43	0.42
3:E:378:GLU:O	3:E:379:THR:C	2.55	0.42
3:E:395:LEU:O	3:E:400:LYS:NZ	2.51	0.42
3:E:153:GLN:NE2	3:E:153:GLN:HA	2.35	0.42
3:E:291:TYR:CZ	3:E:334:LYS:HG2	2.54	0.42
3:E:320:ILE:HD13	3:E:339:LEU:HA	2.00	0.42
3:E:520:TYR:O	3:E:524:ILE:HG13	2.19	0.42
3:F:139:LYS:HG2	3:F:141:TYR:HB3	2.01	0.42
1:A:677:ASN:HB3	1:A:679:LYS:O	2.20	0.42
2:B:73:GLY:HA3	2:B:101:TRP:CH2	2.55	0.42
1:C:535:PHE:C	1:C:535:PHE:CD1	2.93	0.42
1:C:617:GLU:HB2	1:C:620:TYR:OH	2.20	0.42
3:F:109:LEU:HD12	3:F:109:LEU:C	2.40	0.42
3:F:239:TYR:HE1	3:F:243:GLU:OE2	2.02	0.42
1:A:555:LEU:HA	1:A:556:PRO:HD3	1.78	0.42
1:C:486:ALA:O	1:C:490:SER:OG	2.25	0.42
1:C:629:THR:HG23	1:C:630:GLN:N	2.34	0.42
3:E:103:LEU:HD12	3:E:104:LEU:H	1.85	0.42
3:E:352:LEU:HD23	3:E:352:LEU:HA	1.69	0.42
1:A:523:LYS:O	1:A:526:THR:HB	2.20	0.42
1:C:677:ASN:ND2	1:C:682:VAL:HG11	2.35	0.42
3:E:571:VAL:O	3:E:574:ARG:HB3	2.19	0.42
3:F:177:CYS:HB3	3:F:240:PHE:CD1	2.55	0.42
3:F:363:THR:O	3:F:366:GLN:HB2	2.20	0.42
3:F:503:ASN:O	3:F:508:PRO:HD3	2.20	0.42
1:A:684:ILE:O	1:A:686:VAL:HG12	2.20	0.42
2:D:67:GLU:CG	2:D:68:CYS:N	2.76	0.42
3:F:166:ILE:HG13	3:F:168:MET:H	1.84	0.42
3:F:178:LYS:HZ1	3:F:236:PRO:HB3	1.85	0.42
1:A:504:LEU:HD23	1:A:504:LEU:N	2.35	0.41
1:A:664:LYS:HB3	1:A:665:PRO:HD2	2.01	0.41
3:E:252:GLY:C	3:E:253:HIS:CG	2.94	0.41
3:F:255:PHE:HZ	3:F:299:HIS:O	2.03	0.41
3:F:352:LEU:HA	3:F:396:ASP:OD1	2.20	0.41
3:F:477:LEU:HD12	3:F:477:LEU:O	2.20	0.41
3:F:494:LEU:CB	3:F:495:TRP:HA	2.39	0.41
3:E:181:ILE:CG2	3:E:243:GLU:HG2	2.50	0.41
3:E:372:MET:O	3:E:381:ARG:CD	2.52	0.41
3:E:453:VAL:HG23	3:E:454:LEU:N	2.34	0.41
3:F:256:PRO:O	3:F:257:LYS:CB	2.68	0.41
3:F:59:LYS:HD3	3:F:60:ASN:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:HD23	1:A:561:ARG:NH1	2.34	0.41
1:A:579:LEU:HA	1:A:579:LEU:HD23	1.82	0.41
2:B:94:CYS:N	2:B:99:ARG:O	2.49	0.41
2:D:28:ASN:OD1	2:D:28:ASN:N	2.53	0.41
3:E:108:GLU:OE1	3:E:109:LEU:CA	2.68	0.41
3:E:326:ARG:CG	3:E:326:ARG:NH1	2.83	0.41
3:F:248:LEU:HG	3:F:248:LEU:H	1.73	0.41
1:C:474:LEU:HA	1:C:474:LEU:HD23	1.89	0.41
3:E:344:LEU:HD12	3:E:344:LEU:HA	1.65	0.41
3:E:362:LEU:HD23	3:E:362:LEU:HA	1.72	0.41
3:E:83:ARG:O	3:E:86:TYR:N	2.50	0.41
3:F:463:ASP:O	3:F:466:GLN:O	2.37	0.41
1:A:477:GLN:O	1:A:478:ASN:ND2	2.53	0.41
2:B:93:VAL:HG23	2:B:94:CYS:O	2.20	0.41
1:C:520:GLN:HG3	1:C:573:ARG:NH1	2.36	0.41
3:F:301:ASP:OD1	3:F:302:GLN:HG2	2.20	0.41
3:F:310:LEU:HD21	3:F:355:TYR:CZ	2.56	0.41
1:C:449:VAL:O	1:C:452:LYS:HB2	2.20	0.41
2:D:45:CYS:HB3	2:D:83:CYS:SG	2.61	0.41
3:E:196:GLU:HG2	3:E:198:SER:HB3	2.01	0.41
3:F:312:LEU:HA	3:F:312:LEU:HD23	1.85	0.41
3:F:343:LEU:HA	3:F:343:LEU:HD23	1.83	0.41
2:B:93:VAL:HG23	2:B:94:CYS:N	2.35	0.41
3:E:238:ARG:HH11	3:E:238:ARG:HG2	1.86	0.41
3:E:248:LEU:HA	3:E:248:LEU:HD23	1.88	0.41
3:E:258:MET:H	3:E:258:MET:HG2	1.62	0.41
3:E:449:LEU:HD12	3:E:449:LEU:HA	1.87	0.41
1:A:459:LYS:HE3	1:A:459:LYS:HB3	1.82	0.41
1:A:507:MET:HG2	1:A:545:TRP:CE2	2.55	0.41
1:C:579:LEU:HA	2:D:32:LEU:O	2.21	0.41
2:B:55:GLU:CD	3:E:574:ARG:HH21	2.22	0.41
3:F:244:ILE:O	3:F:247:PHE:HB2	2.20	0.41
3:F:316:ASN:OD1	3:F:338:LEU:HD21	2.20	0.41
3:F:443:GLY:HA3	3:F:444:PRO:HD2	1.88	0.41
3:F:478:LEU:HD22	3:F:478:LEU:HA	1.69	0.41
1:A:629:THR:OG1	1:A:631:ILE:HD12	2.20	0.41
1:C:446:LEU:HD23	1:C:446:LEU:HA	1.87	0.41
1:C:620:TYR:HB2	1:C:625:LEU:HD21	2.03	0.41
3:E:191:VAL:HG23	3:E:201:ASN:ND2	2.36	0.41
2:D:49:ILE:HD12	2:D:50:MET:H	1.85	0.41
3:E:180:LEU:HD23	3:E:180:LEU:HA	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:117:GLN:OE1	3:F:120:GLN:HB3	2.21	0.41
3:F:241:ALA:O	3:F:245:ILE:HD12	2.21	0.41
3:E:351:LEU:HD12	3:E:351:LEU:HA	1.87	0.41
3:E:494:LEU:CD1	3:E:495:TRP:CG	3.04	0.41
3:E:130:GLN:NE2	3:E:183:PHE:O	2.54	0.40
3:E:151:TRP:CE2	3:E:214:LYS:HB3	2.56	0.40
3:E:320:ILE:CD1	3:E:339:LEU:HA	2.50	0.40
3:F:166:ILE:CG1	3:F:168:MET:HG2	2.45	0.40
3:F:465:LEU:HD21	3:F:561:ALA:HB2	2.03	0.40
3:F:524:ILE:HD11	3:F:558:LEU:HB2	2.03	0.40
3:E:329:GLU:HG2	3:E:380:LEU:HD11	2.02	0.40
3:E:453:VAL:HG23	3:E:454:LEU:CD2	2.51	0.40
3:F:331:VAL:HG23	3:F:331:VAL:H	1.59	0.40
3:F:444:PRO:HA	3:F:447:ILE:CG1	2.49	0.40
1:C:521:PHE:HD1	1:C:569:PHE:CG	2.39	0.40
3:E:27:GLY:O	3:E:30:GLN:HG3	2.22	0.40
1:A:523:LYS:HE2	1:A:526:THR:HG21	2.03	0.40
1:C:476:HIS:O	1:C:477:GLN:HG2	2.21	0.40
1:C:558:GLU:OE2	1:C:612:LEU:HD22	2.22	0.40
3:E:185:LYS:O	3:E:188:VAL:HG12	2.21	0.40
3:E:194:ASN:HD22	3:E:201:ASN:ND2	2.19	0.40
3:F:137:HIS:NE2	3:F:138:ASN:HB3	2.37	0.40
3:F:375:CYS:HA	3:F:376:PRO:HD3	1.75	0.40
1:C:555:LEU:HA	1:C:556:PRO:HD3	1.81	0.40
3:E:321:GLU:O	3:E:325:GLN:HG2	2.21	0.40
3:F:110:ILE:HG13	3:F:110:ILE:H	1.72	0.40
3:F:157:LEU:HG	3:F:157:LEU:H	1.75	0.40
3:F:318:GLY:O	3:F:321:GLU:HB3	2.22	0.40
3:F:330:SER:OG	3:F:331:VAL:N	2.54	0.40
3:F:295:VAL:HG11	3:F:337:GLU:OE1	2.21	0.40
3:F:516:SER:HB2	3:F:565:PHE:CZ	2.57	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	252/282 (89%)	225 (89%)	26 (10%)	1 (0%)	38	78
1	C	246/282 (87%)	228 (93%)	17 (7%)	1 (0%)	38	78
2	B	80/106 (76%)	72 (90%)	8 (10%)	0	100	100
2	D	83/106 (78%)	76 (92%)	6 (7%)	1 (1%)	15	53
3	E	509/596 (85%)	464 (91%)	44 (9%)	1 (0%)	51	86
3	F	492/596 (83%)	450 (92%)	40 (8%)	2 (0%)	38	78
All	All	1662/1968 (84%)	1515 (91%)	141 (8%)	6 (0%)	38	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	530	PRO
3	E	306	VAL
2	D	65	SER
3	F	113	PRO
1	A	489	ILE
3	F	48	ILE

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	237/258 (92%)	197 (83%)	40 (17%)	2	12
1	C	234/258 (91%)	199 (85%)	35 (15%)	3	16
2	B	74/90 (82%)	60 (81%)	14 (19%)	2	9
2	D	75/90 (83%)	59 (79%)	16 (21%)	1	6
3	E	481/548 (88%)	400 (83%)	81 (17%)	2	12
3	F	471/548 (86%)	391 (83%)	80 (17%)	2	12
All	All	1572/1792 (88%)	1306 (83%)	266 (17%)	2	12

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	LEU
1	A	427	ASP
1	A	429	LEU
1	A	430	LEU
1	A	445	THR
1	A	446	LEU
1	A	454	LYS
1	A	459	LYS
1	A	460	ASP
1	A	461	VAL
1	A	462	PHE
1	A	463	GLN
1	A	474	LEU
1	A	482	ASP
1	A	483	ASP
1	A	490	SER
1	A	508	PHE
1	A	511	ILE
1	A	523	LYS
1	A	526	THR
1	A	527	ASN
1	A	532	ASP
1	A	534	ASP
1	A	536	SER
1	A	538	GLN
1	A	544	SER
1	A	552	THR
1	A	567	THR
1	A	598	ARG
1	A	621	THR
1	A	633	MET
1	A	641	GLN
1	A	645	LYS
1	A	646	SER
1	A	648	LEU
1	A	677	ASN
1	A	679	LYS
1	A	686	VAL
1	A	688	MET
1	A	689	LYS
2	B	20	LYS
2	B	23	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	39	VAL
2	B	53	CYS
2	B	60	GLN
2	B	62	SER
2	B	64	THR
2	B	74	VAL
2	B	77	HIS
2	B	82	HIS
2	B	86	ARG
2	B	91	ARG
2	B	93	VAL
2	B	104	GLN
1	C	431	LYS
1	C	442	LEU
1	C	443	GLU
1	C	447	ASN
1	C	450	MET
1	C	461	VAL
1	C	478	ASN
1	C	481	SER
1	C	483	ASP
1	C	494	GLN
1	C	524	HIS
1	C	525	LEU
1	C	526	THR
1	C	533	LEU
1	C	534	ASP
1	C	549	GLN
1	C	552	THR
1	C	562	SER
1	C	564	GLN
1	C	572	SER
1	C	577	ARG
1	C	596	LYS
1	C	617	GLU
1	C	618	ASP
1	C	621	THR
1	C	626	THR
1	C	633	MET
1	C	634	ASP
1	C	654	GLU
1	C	659	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	661	VAL
1	C	662	GLU
1	C	666	ASP
1	C	682	VAL
1	C	688	MET
2	D	20	LYS
2	D	28	ASN
2	D	37	ILE
2	D	49	ILE
2	D	52	LEU
2	D	53	CYS
2	D	62	SER
2	D	68	CYS
2	D	69	THR
2	D	74	VAL
2	D	86	ARG
2	D	87	TRP
2	D	91	ARG
2	D	92	GLN
2	D	93	VAL
2	D	97	ASP
3	E	1	MET
3	E	3	VAL
3	E	4	GLU
3	E	8	SER
3	E	14	GLN
3	E	31	LEU
3	E	41	HIS
3	E	42	THR
3	E	43	ASP
3	E	44	GLN
3	E	49	ILE
3	E	53	LYS
3	E	54	ASN
3	E	55	LYS
3	E	56	VAL
3	E	77	ASP
3	E	92	LEU
3	E	94	VAL
3	E	102	LEU
3	E	103	LEU
3	E	108	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	116	LYS
3	E	119	SER
3	E	130	GLN
3	E	145	LEU
3	E	149	THR
3	E	155	SER
3	E	156	LEU
3	E	163	LYS
3	E	170	ASP
3	E	184	THR
3	E	190	GLU
3	E	193	ASP
3	E	209	LEU
3	E	216	LEU
3	E	222	THR
3	E	253	HIS
3	E	258	MET
3	E	280	LYS
3	E	281	GLN
3	E	301	ASP
3	E	305	MET
3	E	312	LEU
3	E	326	ARG
3	E	338	LEU
3	E	344	LEU
3	E	354	GLN
3	E	358	ILE
3	E	363	THR
3	E	375	CYS
3	E	398	GLN
3	E	406	CYS
3	E	414	SER
3	E	416	VAL
3	E	432	LEU
3	E	439	LYS
3	E	440	TRP
3	E	442	THR
3	E	455	PHE
3	E	458	GLU
3	E	461	GLU
3	E	462	THR
3	E	465	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	466	GLN
3	E	486	ASN
3	E	490	ASN
3	E	492	THR
3	E	494	LEU
3	E	496	THR
3	E	498	LEU
3	E	500	ASN
3	E	527	SER
3	E	531	GLN
3	E	532	LYS
3	E	535	ASP
3	E	552	GLU
3	E	555	LEU
3	E	557	VAL
3	E	566	ASP
3	E	582	LYS
3	E	583	THR
3	F	8	SER
3	F	18	GLU
3	F	19	GLN
3	F	25	ASP
3	F	31	LEU
3	F	38	GLU
3	F	45	LEU
3	F	46	LEU
3	F	49	ILE
3	F	59	LYS
3	F	61	MET
3	F	85	VAL
3	F	96	LEU
3	F	97	CYS
3	F	107	LEU
3	F	108	GLU
3	F	112	GLU
3	F	116	LYS
3	F	123	LEU
3	F	124	LEU
3	F	125	LEU
3	F	127	GLN
3	F	131	THR
3	F	139	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	166	ILE
3	F	169	ASP
3	F	174	CYS
3	F	180	LEU
3	F	181	ILE
3	F	185	LYS
3	F	188	VAL
3	F	190	GLU
3	F	191	VAL
3	F	192	ILE
3	F	201	ASN
3	F	215	SER
3	F	238	ARG
3	F	249	SER
3	F	279	ASN
3	F	280	LYS
3	F	284	ASP
3	F	289	LEU
3	F	300	ILE
3	F	302	GLN
3	F	326	ARG
3	F	330	SER
3	F	332	ILE
3	F	344	LEU
3	F	348	ASP
3	F	354	GLN
3	F	357	GLU
3	F	377	ILE
3	F	379	THR
3	F	396	ASP
3	F	410	THR
3	F	442	THR
3	F	448	SER
3	F	450	LEU
3	F	452	LEU
3	F	454	LEU
3	F	466	GLN
3	F	478	LEU
3	F	479	ARG
3	F	488	ASN
3	F	491	GLN
3	F	496	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	509	LEU
3	F	510	HIS
3	F	514	ASN
3	F	516	SER
3	F	524	ILE
3	F	531	GLN
3	F	532	LYS
3	F	554	GLN
3	F	560	SER
3	F	562	LEU
3	F	566	ASP
3	F	569	GLU
3	F	580	GLU
3	F	581	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	524	HIS
1	A	548	GLN
1	A	597	ASN
1	A	641	GLN
1	A	677	ASN
2	B	28	ASN
1	C	478	ASN
1	C	527	ASN
1	C	638	GLN
3	E	41	HIS
3	E	152	ASN
3	E	153	GLN
3	E	194	ASN
3	E	253	HIS
3	E	413	HIS
3	E	422	GLN
3	E	445	GLN
3	E	467	ASN
3	F	7	GLN
3	F	14	GLN
3	F	34	GLN
3	F	50	GLN
3	F	60	ASN
3	F	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	120	GLN
3	F	153	GLN
3	F	201	ASN
3	F	224	GLN
3	F	279	ASN
3	F	296	GLN
3	F	302	GLN
3	F	319	HIS
3	F	398	GLN
3	F	422	GLN
3	F	466	GLN
3	F	486	ASN
3	F	488	ASN
3	F	510	HIS

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	258/282 (91%)	-0.09	2 (0%)	86 64	51, 88, 168, 204	0
1	C	254/282 (90%)	0.01	5 (1%)	65 36	60, 99, 174, 207	0
2	B	84/106 (79%)	-0.05	1 (1%)	79 53	52, 114, 156, 217	0
2	D	85/106 (80%)	-0.17	0	100 100	69, 100, 152, 169	0
3	E	523/596 (87%)	-0.10	9 (1%)	70 42	49, 99, 165, 213	0
3	F	512/596 (85%)	-0.08	7 (1%)	75 49	54, 119, 170, 212	0
All	All	1716/1968 (87%)	-0.08	24 (1%)	75 49	49, 104, 169, 217	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	46	LEU	5.4
3	E	488	ASN	3.8
1	C	480	ALA	3.7
3	F	307	LEU	3.1
1	A	549	GLN	3.0
3	E	89	ILE	3.0
1	C	482	ASP	2.8
3	E	52	GLU	2.7
1	C	479	SER	2.6
1	A	458	ASP	2.5
1	C	446	LEU	2.4
3	F	224	GLN	2.4
2	B	63	ALA	2.4
3	E	96	LEU	2.2
3	E	79	GLU	2.2
3	F	253	HIS	2.2
3	E	40	GLY	2.2
3	E	51	ASN	2.2
3	F	50	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	55	LYS	2.1
1	C	451	GLU	2.1
3	F	57	ILE	2.0
3	E	15	ILE	2.0
3	F	18	GLU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ZN	D	201	1/1	0.99	0.20	-0.18	79,79,79,79	0
4	ZN	B	202	1/1	0.99	0.18	-0.43	96,96,96,96	0
4	ZN	D	202	1/1	0.99	0.10	-1.40	120,120,120,120	0
4	ZN	D	203	1/1	0.99	0.19	-	101,101,101,101	0
4	ZN	B	203	1/1	0.98	0.14	-	112,112,112,112	0
4	ZN	B	201	1/1	0.96	0.21	-	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.