



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:38 PM GMT

PDB ID : 4A0K
Title : STRUCTURE OF DDB1-DDB2-CUL4A-RBX1 BOUND TO A 12 BP ABA-SIC SITE CONTAINING DNA-DUPLEX
Authors : Fischer, E.S.; Scrima, A.; Gut, H.; Thoma, N.H.
Deposited on : 2011-09-09
Resolution : 5.93 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

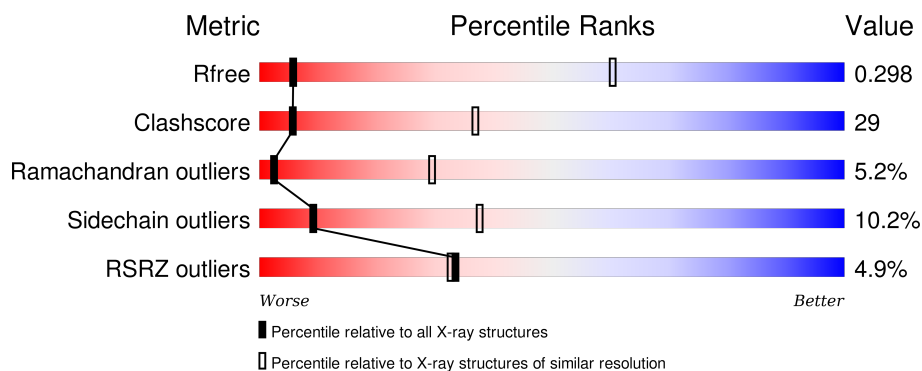
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.93 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}	91344	1001 (8.20-3.66)
Clashscore	102246	1048 (8.00-3.70)
Ramachandran outliers	100387	1022 (8.20-3.66)
Sidechain outliers	100360	1011 (8.20-3.64)
RSRZ outliers	91569	1000 (8.20-3.66)

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	742	 6% 35% 47% 13% . .
2	B	117	 3% 7% 6% . . 82%
3	C	1159	 4% 64% 25% 6% 5%
4	D	382	 3% 75% 15% . . 7%
5	E	12	 33% 75% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	12	<div><div>8%</div><div>50%</div><div>50%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17885 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-4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	719	5809	3692	1007	1076	34	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	EXPRESSION TAG	UNP Q13619
A	19	HIS	-	EXPRESSION TAG	UNP Q13619
A	20	HIS	-	EXPRESSION TAG	UNP Q13619
A	21	HIS	-	EXPRESSION TAG	UNP Q13619
A	22	HIS	-	EXPRESSION TAG	UNP Q13619
A	23	HIS	-	EXPRESSION TAG	UNP Q13619
A	24	HIS	-	EXPRESSION TAG	UNP Q13619
A	25	VAL	-	EXPRESSION TAG	UNP Q13619
A	26	ASP	-	EXPRESSION TAG	UNP Q13619
A	27	GLU	-	EXPRESSION TAG	UNP Q13619
A	28	GLU	-	EXPRESSION TAG	UNP Q13619
A	29	ASN	-	EXPRESSION TAG	UNP Q13619
A	30	LEU	-	EXPRESSION TAG	UNP Q13619
A	31	TYR	-	EXPRESSION TAG	UNP Q13619
A	32	PHE	-	EXPRESSION TAG	UNP Q13619
A	33	GLN	-	EXPRESSION TAG	UNP Q13619
A	34	GLY	-	EXPRESSION TAG	UNP Q13619
A	35	GLY	-	EXPRESSION TAG	UNP Q13619
A	36	GLY	-	EXPRESSION TAG	UNP Q13619
A	37	ARG	-	EXPRESSION TAG	UNP Q13619

- Molecule 2 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBX1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	21	184	126	32	26	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	EXPRESSION TAG	UNP P62877
B	-7	HIS	-	EXPRESSION TAG	UNP P62877
B	-6	HIS	-	EXPRESSION TAG	UNP P62877
B	-5	HIS	-	EXPRESSION TAG	UNP P62877
B	-4	HIS	-	EXPRESSION TAG	UNP P62877
B	-3	HIS	-	EXPRESSION TAG	UNP P62877
B	-2	HIS	-	EXPRESSION TAG	UNP P62877
B	-1	VAL	-	EXPRESSION TAG	UNP P62877
B	0	ASP	-	EXPRESSION TAG	UNP P62877
B	1	GLU	-	EXPRESSION TAG	UNP P62877
B	2	GLU	-	EXPRESSION TAG	UNP P62877
B	3	ASN	-	EXPRESSION TAG	UNP P62877
B	4	LEU	-	EXPRESSION TAG	UNP P62877
B	5	TYR	-	EXPRESSION TAG	UNP P62877
B	6	PHE	-	EXPRESSION TAG	UNP P62877
B	7	GLN	-	EXPRESSION TAG	UNP P62877
B	8	GLY	-	EXPRESSION TAG	UNP P62877
B	9	GLY	-	EXPRESSION TAG	UNP P62877
B	10	GLY	-	EXPRESSION TAG	UNP P62877
B	11	ARG	-	EXPRESSION TAG	UNP P62877

- Molecule 3 is a protein called DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1105	Total	C	N	O	S	0	0	0
			8605	5460	1442	1657	46			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	EXPRESSION TAG	UNP Q16531
C	-17	HIS	-	EXPRESSION TAG	UNP Q16531
C	-16	HIS	-	EXPRESSION TAG	UNP Q16531
C	-15	HIS	-	EXPRESSION TAG	UNP Q16531
C	-14	HIS	-	EXPRESSION TAG	UNP Q16531
C	-13	HIS	-	EXPRESSION TAG	UNP Q16531
C	-12	HIS	-	EXPRESSION TAG	UNP Q16531
C	-11	VAL	-	EXPRESSION TAG	UNP Q16531
C	-10	ASP	-	EXPRESSION TAG	UNP Q16531
C	-9	GLU	-	EXPRESSION TAG	UNP Q16531
C	-8	ASN	-	EXPRESSION TAG	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	EXPRESSION TAG	UNP Q16531
C	-6	TYR	-	EXPRESSION TAG	UNP Q16531
C	-5	PHE	-	EXPRESSION TAG	UNP Q16531
C	-4	GLN	-	EXPRESSION TAG	UNP Q16531
C	-3	GLY	-	EXPRESSION TAG	UNP Q16531
C	-2	GLY	-	EXPRESSION TAG	UNP Q16531
C	-1	GLY	-	EXPRESSION TAG	UNP Q16531
C	0	ARG	-	EXPRESSION TAG	UNP Q16531

- Molecule 4 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	355	Total	C	N	O	S	0	0	0
			2804	1781	491	521	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	76	MET	-	EXPRESSION TAG	UNP Q2YDS1
D	77	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	78	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	79	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	80	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	81	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	82	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	83	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	84	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	85	LEU	-	EXPRESSION TAG	UNP Q2YDS1
D	86	VAL	-	EXPRESSION TAG	UNP Q2YDS1
D	87	PRO	-	EXPRESSION TAG	UNP Q2YDS1
D	88	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	89	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	90	SER	-	EXPRESSION TAG	UNP Q2YDS1
D	91	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	92	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	93	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	180	GLN	LEU	VARIANT	UNP Q2YDS1
D	214	ARG	TRP	VARIANT	UNP Q2YDS1

- Molecule 5 is a DNA chain called 12 BP THF CONTAINING DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	12	Total 234	C 111	N 41	O 70	P 12	0	0	0

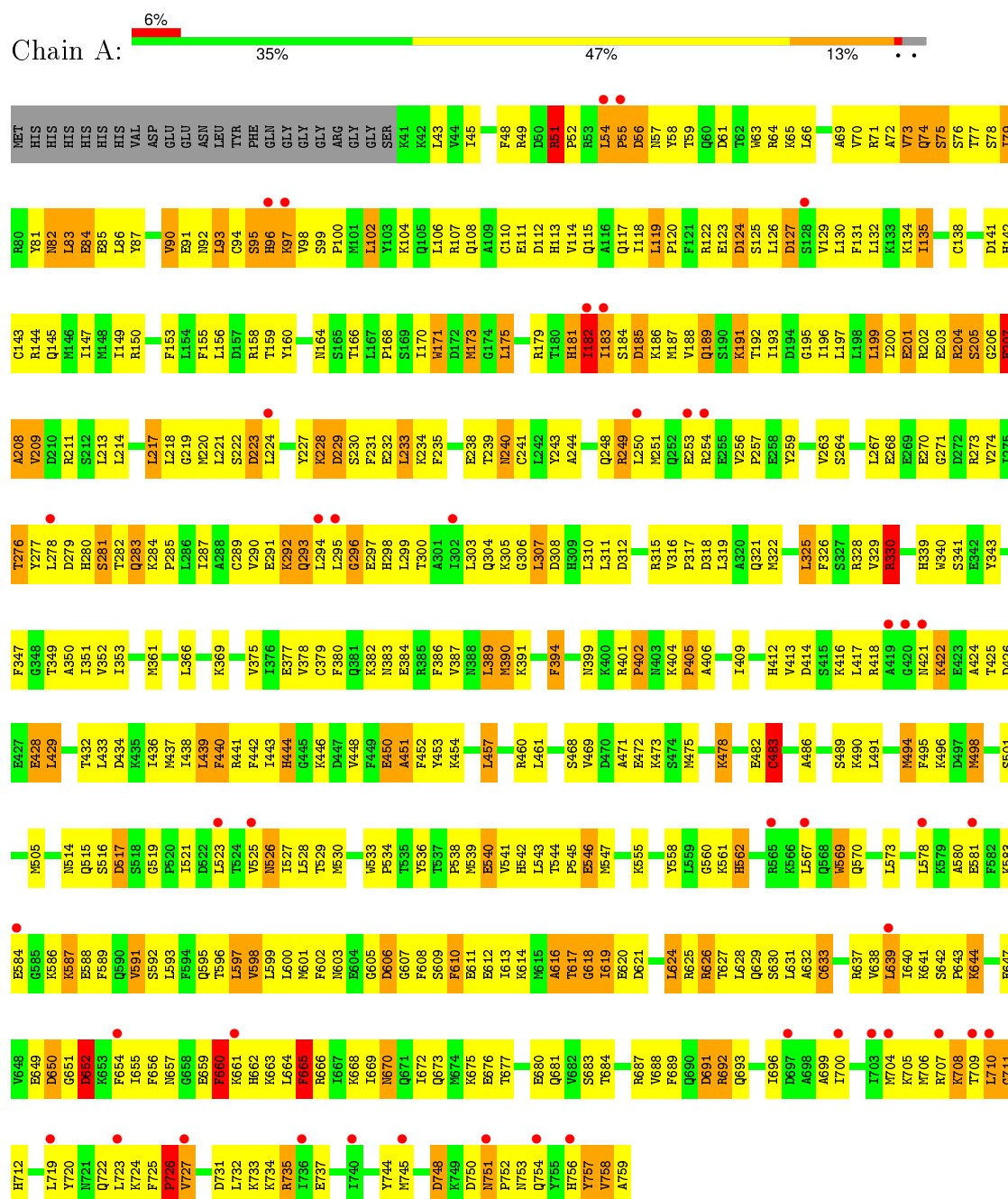
- Molecule 6 is a DNA chain called 12 BP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	12	Total 249	C 118	N 47	O 72	P 12	0	0	0

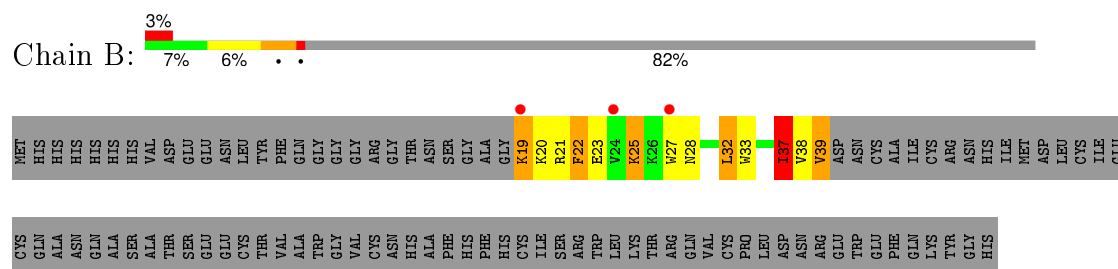
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

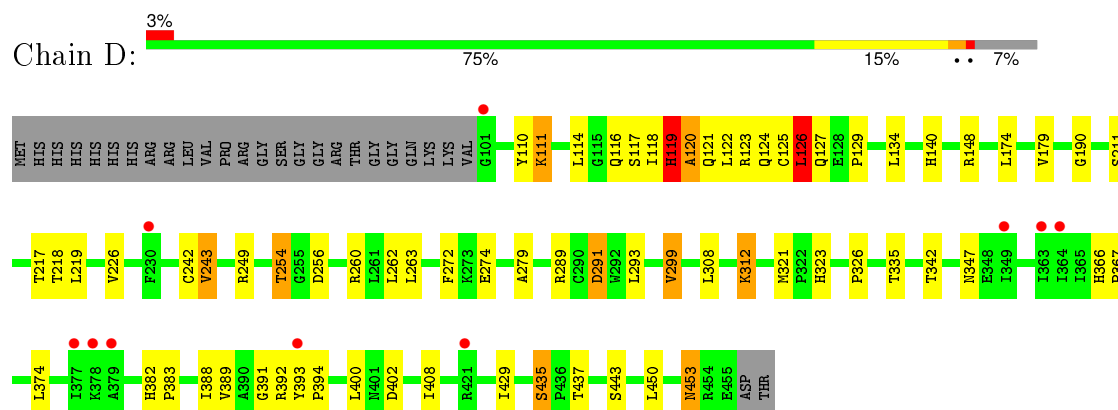
• Molecule 1: CULLIN-4A



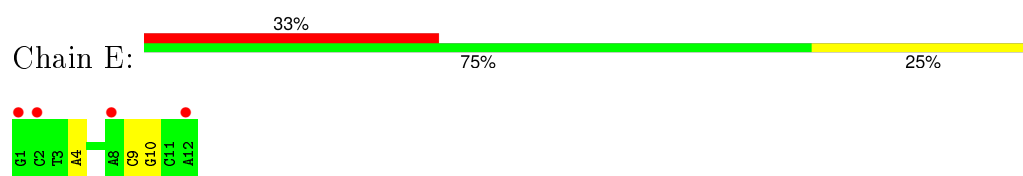
• Molecule 2: E3 UBIQUITIN-PROTEIN LIGASE RBX1



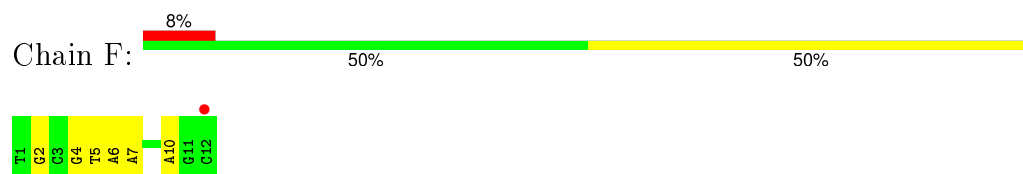
- Molecule 4: DNA DAMAGE-BINDING PROTEIN 2



- Molecule 5: 12 BP THF CONTAINING DNA



- Molecule 6: 12 BP DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.65Å 78.02Å 276.62Å 90.00° 108.50° 90.00°	Depositor
Resolution (Å)	19.98 – 5.93 47.64 – 5.93	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.98-5.93) 98.9 (47.64-5.93)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 6.15Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.269 , 0.270 0.289 , 0.298	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	261.2	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 315.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 11289 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17885	wwPDB-VP
Average B, all atoms (Å ²)	326.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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	0.44	0/5915	0.74	11/7954 (0.1%)
2	B	0.40	0/190	0.48	0/257
3	C	0.46	5/8762 (0.1%)	0.67	9/11875 (0.1%)
4	D	0.37	0/2877	0.58	0/3912
5	E	0.93	1/248 (0.4%)	1.12	0/377
6	F	0.89	0/279	1.36	1/429 (0.2%)
All	All	0.46	6/18271 (0.0%)	0.70	21/24804 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	354	THR	C-N	-11.77	1.06	1.34
3	C	582	LEU	C-N	6.64	1.45	1.33
3	C	13	THR	C-N	6.59	1.49	1.34
3	C	706	GLU	C-N	-5.68	1.21	1.34
5	E	9	DC	C1'-N1	5.59	1.56	1.49
3	C	903	CYS	CB-SG	-5.18	1.73	1.81

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	HIS	CB-CA-C	-10.74	88.92	110.40
1	A	182	ILE	N-CA-C	9.33	136.18	111.00
1	A	181	HIS	CB-CA-C	7.11	124.62	110.40
3	C	624	SER	N-CA-C	7.02	129.96	111.00
1	A	48	PHE	N-CA-C	-6.88	92.43	111.00
3	C	688	PRO	N-CA-C	6.59	129.22	112.10
3	C	689	ASP	N-CA-C	-6.45	93.58	111.00
6	F	2	DG	O4'-C1'-N9	6.33	112.43	108.00
1	A	182	ILE	N-CA-CB	-5.97	97.07	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	CB-CA-C	-5.95	98.51	110.40
3	C	688	PRO	CA-N-CD	-5.90	103.24	111.50
3	C	624	SER	CB-CA-C	-5.85	98.99	110.10
3	C	1139	ILE	N-CA-CB	5.58	123.64	110.80
3	C	354	THR	O-C-N	5.52	131.53	122.70
1	A	637	ARG	N-CA-C	5.46	125.74	111.00
1	A	296	GLY	N-CA-C	-5.43	99.52	113.10
1	A	665	PHE	N-CA-C	-5.37	96.50	111.00
1	A	74	GLN	N-CA-C	-5.36	96.53	111.00
1	A	73	VAL	N-CA-C	-5.28	96.75	111.00
3	C	523	PRO	CA-N-CD	-5.25	104.14	111.50
3	C	422	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

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	5809	0	5796	617	0
2	B	184	0	192	29	0
3	C	8605	0	8542	369	1
4	D	2804	0	2720	45	0
5	E	234	0	132	3	0
6	F	249	0	136	7	0
All	All	17885	0	17518	1034	1

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 (1034) 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:131:PHE:CZ	1:A:188:VAL:HA	1.63	1.33
1:A:696:ILE:CD1	1:A:723:LEU:HG	1.57	1.33

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:CD1	1:A:181:HIS:HB3	1.60	1.29
1:A:135:ILE:HD11	1:A:188:VAL:CG1	1.63	1.26
1:A:696:ILE:HD13	1:A:723:LEU:CD1	1.69	1.21
1:A:696:ILE:HD13	1:A:723:LEU:CG	1.71	1.20
1:A:135:ILE:CD1	1:A:188:VAL:CG1	2.21	1.19
1:A:118:ILE:HD11	1:A:181:HIS:CB	1.73	1.16
1:A:131:PHE:CZ	1:A:188:VAL:HG13	1.79	1.15
1:A:118:ILE:HD11	1:A:181:HIS:HB3	1.20	1.15
1:A:699:ALA:HB1	1:A:722:GLN:NE2	1.63	1.13
1:A:692:ARG:CB	1:A:725:PHE:CE2	2.32	1.12
1:A:118:ILE:HD11	1:A:181:HIS:CG	1.84	1.12
1:A:183:ILE:HD11	1:A:220:MET:CE	1.83	1.08
1:A:43:LEU:HD11	3:C:400:ALA:HB1	1.17	1.08
1:A:131:PHE:HZ	1:A:188:VAL:CA	1.67	1.07
1:A:69:ALA:HA	1:A:79:ILE:HG21	1.33	1.07
2:B:37:ILE:HD13	2:B:38:VAL:N	1.69	1.07
2:B:25:LYS:HE3	2:B:25:LYS:HA	1.30	1.07
1:A:692:ARG:HB3	1:A:725:PHE:CE2	1.89	1.06
1:A:692:ARG:HB2	1:A:725:PHE:CZ	1.90	1.05
1:A:107:ARG:NH1	1:A:173:MET:HG3	1.70	1.05
1:A:129:VAL:HG13	1:A:130:LEU:N	1.71	1.04
2:B:37:ILE:HG12	2:B:38:VAL:H	1.20	1.04
1:A:700:ILE:HD13	1:A:719:LEU:HD21	1.38	1.04
1:A:129:VAL:CG1	1:A:130:LEU:H	1.72	1.03
1:A:135:ILE:HD11	1:A:188:VAL:HG11	1.04	1.03
3:C:539:ALA:HB2	3:C:561:TRP:CD1	1.94	1.02
2:B:37:ILE:CG1	2:B:38:VAL:H	1.71	1.02
3:C:562:THR:O	3:C:564:ILE:HG13	1.61	1.01
2:B:37:ILE:HD13	2:B:37:ILE:C	1.80	1.01
3:C:185:PRO:HD3	4:D:289:ARG:HB3	1.40	1.01
1:A:131:PHE:CZ	1:A:188:VAL:CA	2.44	1.00
1:A:692:ARG:HB2	1:A:725:PHE:CE2	1.94	0.99
3:C:539:ALA:HB2	3:C:561:TRP:HD1	1.26	0.99
1:A:626:ARG:HA	1:A:629:GLN:HB2	1.41	0.99
1:A:705:LYS:HB2	1:A:757:TYR:CE2	1.98	0.99
3:C:185:PRO:CD	4:D:289:ARG:HB3	1.93	0.99
1:A:422:LYS:HB3	1:A:422:LYS:NZ	1.77	0.98
1:A:700:ILE:CD1	1:A:719:LEU:HD21	1.93	0.98
1:A:642:SER:HB2	1:A:643:PRO:HD3	1.46	0.97
1:A:696:ILE:HD13	1:A:723:LEU:HD11	1.44	0.97
1:A:657:ASN:HD21	1:A:659:GLU:HB2	1.28	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:ILE:HD13	1:A:723:LEU:HG	1.32	0.96
1:A:74:GLN:HE22	1:A:110:CYS:HA	1.31	0.96
1:A:491:LEU:HA	1:A:494:MET:HG3	1.48	0.96
1:A:197:LEU:CD2	1:A:235:PHE:HA	1.96	0.96
1:A:705:LYS:HA	1:A:757:TYR:CD2	2.01	0.95
1:A:638:VAL:HG12	1:A:639:LEU:HD23	1.48	0.95
3:C:465:HIS:ND1	3:C:523:PRO:HD3	1.82	0.95
3:C:329:GLY:HA3	3:C:384:GLU:HG2	1.45	0.95
2:B:37:ILE:CD1	2:B:38:VAL:N	2.30	0.94
1:A:131:PHE:HZ	1:A:188:VAL:HA	1.13	0.94
1:A:183:ILE:HD11	1:A:220:MET:HE3	1.49	0.93
1:A:131:PHE:CE1	1:A:191:LYS:HD3	2.04	0.93
1:A:118:ILE:CG1	1:A:181:HIS:HB3	1.98	0.93
1:A:183:ILE:HD11	1:A:220:MET:SD	2.09	0.93
2:B:37:ILE:CG1	2:B:38:VAL:N	2.30	0.92
1:A:122:ARG:HD2	1:A:186:LYS:HZ2	1.34	0.91
1:A:696:ILE:HD11	1:A:723:LEU:HG	1.51	0.91
1:A:197:LEU:HD22	1:A:235:PHE:HA	1.50	0.91
1:A:131:PHE:HZ	1:A:188:VAL:CB	1.84	0.91
3:C:507:GLN:NE2	3:C:552:LEU:HA	1.85	0.91
2:B:19:LYS:HA	2:B:19:LYS:HE3	1.53	0.91
1:A:82:ASN:OD1	1:A:85:GLU:HG3	1.69	0.90
1:A:51:ARG:O	1:A:51:ARG:HG2	1.72	0.90
1:A:196:ILE:HD13	1:A:218:LEU:HD21	1.53	0.90
1:A:63:TRP:CZ3	1:A:102:LEU:HA	2.07	0.90
1:A:129:VAL:CG1	1:A:130:LEU:N	2.30	0.90
3:C:356:LEU:HD21	3:C:712:ILE:HD13	1.52	0.90
3:C:465:HIS:CE1	3:C:523:PRO:HD3	2.07	0.90
3:C:18:CYS:HB2	3:C:313:CYS:SG	2.12	0.90
1:A:131:PHE:CZ	1:A:188:VAL:CG1	2.54	0.89
1:A:745:MET:HA	1:A:757:TYR:O	1.71	0.89
1:A:43:LEU:CD1	3:C:400:ALA:HB1	2.03	0.89
1:A:99:SER:HB2	1:A:100:PRO:HD3	1.53	0.88
1:A:696:ILE:CD1	1:A:723:LEU:CG	2.35	0.88
1:A:106:LEU:HD22	1:A:153:PHE:CE2	2.09	0.87
3:C:578:HIS:CD2	3:C:623:LEU:HD12	2.09	0.87
4:D:323:HIS:NE2	4:D:342:THR:HG21	1.88	0.87
1:A:538:PRO:HA	1:A:570:GLN:HE22	1.40	0.87
1:A:70:VAL:HG21	1:A:106:LEU:CD1	2.05	0.87
3:C:649:VAL:HG12	3:C:650:PHE:H	1.39	0.86
1:A:196:ILE:HD13	1:A:218:LEU:CD2	2.06	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:VAL:HA	1:A:278:LEU:HB2	1.57	0.86
1:A:605:GLY:O	1:A:606:ASP:HB2	1.75	0.86
1:A:131:PHE:CD1	1:A:191:LYS:HD3	2.11	0.86
1:A:144:ARG:HA	1:A:147:ILE:HD12	1.58	0.86
1:A:63:TRP:CH2	1:A:102:LEU:HA	2.11	0.85
3:C:711:HIS:CG	3:C:712:ILE:N	2.43	0.85
3:C:23:PHE:H	3:C:30:ASN:HD22	1.21	0.85
1:A:122:ARG:NE	1:A:186:LYS:HZ3	1.74	0.85
3:C:165:ILE:HD11	3:C:188:ARG:NH2	1.92	0.85
1:A:199:LEU:HD12	1:A:214:LEU:HD11	1.59	0.85
1:A:213:LEU:O	1:A:217:LEU:HD12	1.76	0.85
3:C:81:THR:HG21	3:C:85:ASN:HD22	1.41	0.84
1:A:422:LYS:HB3	1:A:422:LYS:HZ2	1.38	0.84
1:A:115:GLN:HG2	1:A:181:HIS:CE1	2.14	0.83
1:A:696:ILE:HA	1:A:723:LEU:HD11	1.60	0.83
3:C:707:ILE:HG23	3:C:708:GLN:N	1.92	0.83
1:A:119:LEU:HB2	1:A:120:PRO:HD3	1.60	0.83
3:C:446:THR:HG22	3:C:447:GLU:H	1.43	0.83
3:C:520:GLN:HG3	3:C:529:ILE:HG13	1.60	0.82
1:A:135:ILE:CD1	1:A:188:VAL:HG13	2.06	0.82
1:A:581:GLU:HB2	2:B:21:ARG:HA	1.62	0.82
3:C:482:GLU:CD	3:C:483:PRO:HD3	2.00	0.81
1:A:705:LYS:HB2	1:A:757:TYR:HE2	1.45	0.81
1:A:93:LEU:O	1:A:93:LEU:HD22	1.79	0.81
1:A:699:ALA:CB	1:A:722:GLN:NE2	2.43	0.81
2:B:38:VAL:O	2:B:38:VAL:HG12	1.80	0.81
3:C:413:LEU:HB2	3:C:424:THR:HB	1.62	0.81
3:C:507:GLN:HE22	3:C:553:SER:H	1.25	0.81
1:A:757:TYR:HE1	1:A:759:ALA:HA	1.47	0.80
3:C:708:GLN:NE2	3:C:708:GLN:HA	1.94	0.80
1:A:284:LYS:HB3	1:A:285:PRO:HD3	1.61	0.80
1:A:131:PHE:HZ	1:A:188:VAL:CG1	1.93	0.80
1:A:366:LEU:HD23	1:A:439:LEU:HD12	1.62	0.80
1:A:131:PHE:CE2	1:A:188:VAL:HG13	2.16	0.80
3:C:534:MET:HE2	3:C:569:LEU:HD11	1.62	0.80
1:A:680:GLU:O	1:A:684:THR:HG22	1.81	0.80
1:A:296:GLY:O	1:A:297:GLU:HB2	1.82	0.79
3:C:509:VAL:HG23	3:C:543:ILE:HD13	1.62	0.79
1:A:705:LYS:CA	1:A:757:TYR:CD2	2.65	0.79
1:A:93:LEU:CD2	1:A:93:LEU:O	2.30	0.79
1:A:122:ARG:NE	1:A:186:LYS:NZ	2.30	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LEU:HD21	1:A:631:LEU:HD12	1.64	0.79
1:A:211:ARG:HD2	1:A:276:THR:HG21	1.64	0.79
3:C:182:TYR:O	3:C:188:ARG:CB	2.30	0.79
1:A:696:ILE:HD11	1:A:725:PHE:CZ	2.18	0.78
1:A:204:ARG:HH21	1:A:270:GLU:CD	1.86	0.78
3:C:412:PRO:HB2	3:C:422:ASP:OD2	1.83	0.78
3:C:185:PRO:CG	4:D:289:ARG:CB	2.62	0.78
1:A:692:ARG:O	1:A:696:ILE:HG12	1.84	0.78
1:A:138:CYS:SG	1:A:182:ILE:CD1	2.71	0.77
1:A:175:LEU:HD12	1:A:223:ASP:O	1.85	0.77
1:A:461:LEU:HB3	1:A:498:MET:HE2	1.65	0.77
1:A:704:MET:C	1:A:757:TYR:HD2	1.86	0.77
3:C:649:VAL:HG12	3:C:650:PHE:N	2.00	0.77
1:A:527:ILE:HD11	1:A:567:LEU:HD22	1.65	0.77
1:A:274:VAL:HG11	1:A:283:GLN:HE21	1.49	0.77
3:C:185:PRO:HG3	4:D:289:ARG:HB2	1.65	0.77
1:A:129:VAL:HG13	1:A:130:LEU:H	1.32	0.77
3:C:578:HIS:NE2	3:C:623:LEU:HD12	1.99	0.77
3:C:602:LEU:C	3:C:603:LEU:HD23	2.04	0.76
1:A:186:LYS:HB3	1:A:188:VAL:HG23	1.67	0.76
3:C:23:PHE:H	3:C:30:ASN:ND2	1.83	0.76
1:A:603:ASN:OD1	2:B:22:PHE:HB2	1.86	0.76
3:C:452:VAL:HG12	3:C:454:ASP:OD1	1.86	0.75
1:A:329:VAL:HG12	1:A:330:ARG:H	1.49	0.75
1:A:601:MET:HE1	1:A:616:ALA:CB	2.17	0.75
1:A:597:LEU:HB3	1:A:617:THR:HG21	1.68	0.75
1:A:276:THR:HG22	1:A:277:TYR:N	2.02	0.75
1:A:578:LEU:HD11	1:A:596:THR:HG23	1.67	0.75
3:C:450:GLY:HA3	3:C:479:VAL:CG2	2.17	0.75
3:C:448:LEU:HB3	3:C:451:PHE:HD2	1.52	0.74
3:C:507:GLN:HE22	3:C:552:LEU:HA	1.49	0.74
3:C:469:ILE:HD11	3:C:476:VAL:HG23	1.69	0.74
3:C:389:ILE:HD13	3:C:713:ARG:HG2	1.68	0.74
3:C:185:PRO:CG	4:D:289:ARG:HB2	2.17	0.74
1:A:705:LYS:O	1:A:708:LYS:NZ	2.21	0.74
1:A:279:ASP:OD1	1:A:281:SER:HB3	1.87	0.74
1:A:595:GLN:HE22	1:A:669:ILE:HG22	1.53	0.74
1:A:316:VAL:HB	1:A:317:PRO:HD3	1.70	0.74
1:A:688:VAL:O	1:A:692:ARG:HG3	1.88	0.73
1:A:696:ILE:O	1:A:700:ILE:HG12	1.88	0.73
1:A:122:ARG:CD	1:A:186:LYS:NZ	2.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD22	1:A:153:PHE:CZ	2.22	0.73
3:C:451:PHE:CD1	3:C:470:GLN:HB2	2.24	0.73
1:A:294:LEU:O	1:A:295:LEU:HD23	1.86	0.73
1:A:630:SER:HB3	1:A:672:ILE:HD11	1.70	0.73
3:C:578:HIS:CD2	3:C:623:LEU:H	2.06	0.73
1:A:609:SER:O	1:A:612:GLU:HG2	1.87	0.73
1:A:77:THR:HG22	1:A:78:SER:H	1.53	0.73
3:C:1055:GLN:HE22	3:C:1090:ASP:H	1.37	0.73
1:A:118:ILE:HG12	1:A:181:HIS:HB3	1.71	0.73
3:C:465:HIS:O	3:C:467:GLN:HG3	1.89	0.72
1:A:138:CYS:SG	1:A:182:ILE:HD13	2.29	0.72
1:A:135:ILE:HD12	1:A:188:VAL:HG13	1.70	0.72
3:C:184:ASP:HB2	3:C:185:PRO:HD2	1.70	0.72
1:A:529:THR:HA	2:B:33:TRP:NE1	2.03	0.72
3:C:657:THR:HG22	3:C:658:VAL:H	1.54	0.72
1:A:340:TRP:CH2	1:A:390:MET:HB2	2.25	0.72
1:A:240:ASN:OD1	1:A:289:CYS:HB3	1.90	0.72
3:C:465:HIS:HB2	3:C:467:GLN:HE21	1.55	0.72
1:A:49:ARG:HD2	1:A:51:ARG:NH2	2.05	0.72
1:A:208:ALA:O	1:A:209:VAL:CB	2.38	0.72
3:C:469:ILE:HD13	3:C:470:GLN:N	2.05	0.72
1:A:601:MET:HE1	1:A:616:ALA:HB3	1.72	0.71
3:C:182:TYR:O	3:C:188:ARG:HB2	1.89	0.71
1:A:239:THR:C	1:A:241:CYS:H	1.91	0.71
4:D:263:LEU:HB2	4:D:272:PHE:HB3	1.73	0.71
1:A:660:PHE:O	1:A:662:HIS:N	2.23	0.71
3:C:329:GLY:HA3	3:C:384:GLU:CG	2.20	0.71
1:A:601:MET:CE	1:A:616:ALA:CB	2.68	0.71
3:C:889:ARG:HD3	3:C:901:THR:HB	1.73	0.71
1:A:118:ILE:HD11	1:A:181:HIS:ND1	2.06	0.71
3:C:185:PRO:CG	4:D:289:ARG:HB3	2.21	0.71
1:A:432:THR:O	1:A:436:ILE:HG13	1.91	0.71
1:A:602:PHE:HD2	1:A:656:PHE:HB2	1.54	0.70
3:C:561:TRP:O	3:C:587:ILE:CG2	2.40	0.70
1:A:643:PRO:CD	1:A:652:ASP:HA	2.21	0.70
3:C:704:ILE:O	3:C:705:ASP:HB2	1.91	0.70
3:C:451:PHE:CE1	3:C:470:GLN:HB2	2.25	0.70
3:C:396:ILE:HA	3:C:704:ILE:O	1.90	0.70
3:C:592:LEU:HD23	3:C:593:MET:O	1.92	0.70
1:A:204:ARG:NH2	1:A:270:GLU:OE1	2.23	0.70
1:A:578:LEU:HD13	1:A:591:VAL:CG2	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG12	1:A:130:LEU:H	1.55	0.70
1:A:122:ARG:HD2	1:A:186:LYS:NZ	2.06	0.70
1:A:705:LYS:CB	1:A:757:TYR:CE2	2.73	0.70
1:A:587:LYS:H	1:A:587:LYS:HD2	1.57	0.69
3:C:399:HIS:NE2	3:C:703:THR:HG22	2.07	0.69
1:A:692:ARG:O	1:A:725:PHE:HZ	1.76	0.69
3:C:706:GLU:OE1	3:C:706:GLU:HA	1.90	0.69
3:C:652:CYS:HB3	3:C:676:VAL:O	1.91	0.69
1:A:329:VAL:HG12	1:A:330:ARG:N	2.08	0.69
3:C:480:SER:O	3:C:484:LYS:HA	1.92	0.69
3:C:532:THR:HG22	3:C:533:GLU:N	2.06	0.69
1:A:619:ILE:HG22	1:A:620:GLU:H	1.56	0.69
3:C:618:ILE:HG13	3:C:619:GLU:N	2.08	0.68
3:C:452:VAL:HG23	3:C:470:GLN:OE1	1.93	0.68
3:C:536:HIS:CD2	3:C:563:ASP:HB3	2.29	0.68
1:A:560:GLY:O	1:A:561:LYS:HB2	1.93	0.68
1:A:751:ASN:O	1:A:753:ASN:N	2.27	0.68
3:C:722:ARG:NH2	3:C:812:TYR:OH	2.26	0.68
1:A:204:ARG:CZ	1:A:243:TYR:HE2	2.07	0.68
3:C:450:GLY:HA3	3:C:479:VAL:HG21	1.74	0.68
3:C:440:GLY:O	3:C:686:GLY:HA3	1.94	0.68
3:C:1051:LEU:HB2	3:C:1089:ILE:HD13	1.76	0.68
1:A:122:ARG:CD	1:A:186:LYS:HZ2	2.06	0.68
1:A:555:LYS:HD2	1:A:569:TRP:HZ3	1.58	0.67
1:A:70:VAL:HG21	1:A:106:LEU:HD11	1.77	0.67
1:A:630:SER:CB	1:A:672:ILE:HD11	2.24	0.67
3:C:596:PHE:HE1	3:C:648:ASN:HA	1.58	0.67
3:C:711:HIS:CG	3:C:712:ILE:H	2.08	0.67
1:A:249:ARG:O	1:A:253:GLU:HB2	1.95	0.67
1:A:630:SER:O	1:A:631:LEU:HB2	1.94	0.67
1:A:63:TRP:CH2	1:A:102:LEU:CA	2.77	0.67
1:A:82:ASN:O	1:A:83:LEU:C	2.33	0.67
3:C:165:ILE:CD1	3:C:188:ARG:NH2	2.58	0.67
1:A:63:TRP:NE1	1:A:93:LEU:HD11	2.10	0.66
1:A:274:VAL:HG11	1:A:283:GLN:HB2	1.76	0.66
3:C:460:CYS:HA	3:C:469:ILE:O	1.95	0.66
1:A:593:LEU:HD21	2:B:27:TRP:HE1	1.60	0.66
1:A:183:ILE:CD1	1:A:220:MET:SD	2.84	0.66
1:A:49:ARG:HD2	1:A:51:ARG:HH21	1.60	0.66
1:A:409:ILE:HG13	1:A:443:ILE:CD1	2.26	0.66
1:A:705:LYS:N	1:A:757:TYR:HD2	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PRO:CA	1:A:570:GLN:HE22	2.08	0.66
1:A:79:ILE:H	1:A:79:ILE:HD12	1.59	0.66
3:C:189:HIS:HB3	3:C:210:GLU:O	1.95	0.66
1:A:696:ILE:HD11	1:A:725:PHE:CE1	2.31	0.66
3:C:582:LEU:O	3:C:583:GLY:O	2.14	0.66
1:A:118:ILE:CG2	1:A:186:LYS:HE3	2.25	0.66
3:C:711:HIS:O	3:C:712:ILE:HG13	1.95	0.66
3:C:507:GLN:HE22	3:C:553:SER:N	1.94	0.66
1:A:366:LEU:CD2	1:A:439:LEU:HD12	2.25	0.65
4:D:443:SER:HB2	4:D:450:LEU:HB2	1.77	0.65
1:A:74:GLN:HE22	1:A:110:CYS:CA	2.07	0.65
1:A:709:THR:O	1:A:710:LEU:HB2	1.95	0.65
1:A:83:LEU:O	1:A:84:GLU:C	2.35	0.65
1:A:688:VAL:O	1:A:692:ARG:CG	2.45	0.65
3:C:520:GLN:HG3	3:C:529:ILE:CG1	2.27	0.65
3:C:184:ASP:O	3:C:187:GLY:N	2.30	0.65
1:A:251:MET:HA	1:A:251:MET:CE	2.27	0.65
1:A:96:HIS:O	1:A:97:LYS:CB	2.44	0.65
1:A:69:ALA:O	1:A:73:VAL:HG23	1.97	0.65
1:A:734:LYS:HA	1:A:737:GLU:CD	2.18	0.65
3:C:562:THR:O	3:C:564:ILE:N	2.30	0.65
3:C:188:ARG:C	3:C:189:HIS:CG	2.71	0.65
1:A:84:GLU:O	1:A:87:TYR:N	2.29	0.64
4:D:119:HIS:O	4:D:122:LEU:N	2.30	0.64
3:C:601:TYR:CE2	3:C:666:LEU:HD21	2.32	0.64
1:A:54:LEU:CB	1:A:55:PRO:HD3	2.27	0.64
1:A:312:ASP:HB3	1:A:343:TYR:OH	1.97	0.64
3:C:188:ARG:C	3:C:189:HIS:CD2	2.71	0.64
1:A:183:ILE:HG21	1:A:221:LEU:HD23	1.78	0.64
1:A:249:ARG:HH11	1:A:249:ARG:HB3	1.62	0.64
1:A:630:SER:C	1:A:632:ALA:H	2.01	0.64
3:C:507:GLN:NE2	3:C:553:SER:H	1.94	0.64
2:B:25:LYS:CE	2:B:25:LYS:HA	2.15	0.64
1:A:642:SER:CB	1:A:643:PRO:HD3	2.24	0.64
4:D:125:CYS:O	4:D:127:GLN:N	2.30	0.64
3:C:926:LEU:CD2	4:D:129:PRO:HG3	2.28	0.64
1:A:94:CYS:SG	1:A:156:LEU:HD13	2.37	0.64
1:A:707:ARG:CD	1:A:710:LEU:HD22	2.28	0.64
3:C:184:ASP:O	3:C:186:GLN:N	2.31	0.63
4:D:124:GLN:O	4:D:124:GLN:CG	2.45	0.63
1:A:197:LEU:HD21	1:A:235:PHE:HA	1.78	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:119:HIS:O	4:D:120:ALA:C	2.36	0.63
1:A:705:LYS:CA	1:A:757:TYR:CE2	2.82	0.63
1:A:705:LYS:N	1:A:757:TYR:CD2	2.67	0.63
1:A:422:LYS:HB3	1:A:422:LYS:HZ3	1.63	0.63
1:A:292:LYS:HD2	1:A:292:LYS:O	1.99	0.63
1:A:183:ILE:HG21	1:A:221:LEU:CD2	2.28	0.63
3:C:414:ARG:CB	3:C:462:ASN:HD21	2.12	0.63
1:A:404:LYS:N	1:A:405:PRO:HD2	2.14	0.63
4:D:249:ARG:HE	4:D:291:ASP:HB3	1.64	0.63
1:A:108:GLN:HA	1:A:111:GLU:HB3	1.81	0.63
2:B:37:ILE:C	2:B:37:ILE:CD1	2.54	0.63
1:A:122:ARG:CZ	1:A:186:LYS:NZ	2.61	0.63
1:A:118:ILE:HG23	1:A:186:LYS:HE3	1.80	0.62
1:A:700:ILE:HD13	1:A:719:LEU:CD2	2.23	0.62
3:C:482:GLU:OE1	3:C:483:PRO:HD3	2.00	0.62
3:C:518:TYR:HD1	3:C:519:LEU:N	1.95	0.62
1:A:523:LEU:HD11	1:A:525:VAL:HG22	1.81	0.62
1:A:77:THR:HG22	1:A:78:SER:N	2.13	0.62
1:A:757:TYR:O	1:A:758:VAL:HB	1.99	0.62
3:C:446:THR:CG2	3:C:447:GLU:H	2.06	0.62
3:C:591:ILE:O	3:C:592:LEU:HB2	2.00	0.62
1:A:369:LYS:HE2	1:A:390:MET:HE3	1.82	0.62
3:C:657:THR:HG21	3:C:668:PHE:HB3	1.82	0.62
1:A:726:PRO:O	1:A:727:VAL:HB	2.00	0.62
3:C:399:HIS:CE1	3:C:703:THR:HG22	2.34	0.62
1:A:609:SER:H	1:A:612:GLU:CD	2.03	0.62
3:C:476:VAL:HG13	3:C:490:TRP:HB3	1.81	0.61
1:A:692:ARG:O	1:A:725:PHE:CZ	2.52	0.61
1:A:66:LEU:HD23	1:A:86:LEU:HD22	1.81	0.61
1:A:126:LEU:O	1:A:127:ASP:CG	2.38	0.61
1:A:57:ASN:O	1:A:59:THR:N	2.27	0.61
5:E:10:DG:N2	6:F:4:DG:C2	2.69	0.61
1:A:310:LEU:HD22	1:A:315:ARG:HB2	1.81	0.61
3:C:562:THR:HG22	3:C:563:ASP:N	2.16	0.61
1:A:228:LYS:HD3	1:A:232:GLU:HG2	1.81	0.61
1:A:132:LEU:HD21	1:A:192:THR:HA	1.83	0.61
1:A:203:GLU:C	1:A:205:SER:H	2.03	0.61
1:A:409:ILE:O	1:A:413:VAL:HG23	2.00	0.61
4:D:127:GLN:O	4:D:127:GLN:HG2	2.00	0.61
3:C:7:VAL:HG13	3:C:1091:GLY:HA3	1.81	0.61
1:A:183:ILE:HD13	1:A:221:LEU:HD23	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:ILE:CD1	1:A:723:LEU:CD1	2.63	0.61
1:A:624:LEU:CD2	1:A:628:LEU:HG	2.30	0.61
1:A:570:GLN:HG2	2:B:32:LEU:HD11	1.81	0.61
3:C:617:ASN:HD21	3:C:619:GLU:HB2	1.64	0.61
3:C:582:LEU:HD13	3:C:583:GLY:H	1.65	0.61
1:A:131:PHE:CD1	1:A:191:LYS:CD	2.84	0.61
1:A:689:PHE:O	1:A:693:GLN:NE2	2.33	0.61
3:C:927:MET:SD	4:D:129:PRO:HB2	2.41	0.61
1:A:640:ILE:O	1:A:654:PHE:HA	2.01	0.61
3:C:492:GLU:HG3	3:C:496:LYS:HB2	1.83	0.61
1:A:83:LEU:O	1:A:86:LEU:N	2.30	0.60
1:A:276:THR:HG22	1:A:277:TYR:H	1.67	0.60
1:A:340:TRP:HH2	1:A:390:MET:HB2	1.65	0.60
1:A:724:LYS:HE2	1:A:724:LYS:HA	1.82	0.60
3:C:446:THR:HG22	3:C:447:GLU:N	2.16	0.60
1:A:486:ALA:HA	1:A:489:SER:HB2	1.83	0.60
1:A:73:VAL:HG12	1:A:145:GLN:HB2	1.84	0.60
1:A:707:ARG:HD2	1:A:710:LEU:HD22	1.84	0.60
1:A:538:PRO:HA	1:A:570:GLN:NE2	2.12	0.60
3:C:889:ARG:HG3	3:C:904:ASN:ND2	2.16	0.60
3:C:167:VAL:HG13	3:C:180:PHE:HB3	1.84	0.60
1:A:527:ILE:HD11	1:A:567:LEU:CD2	2.31	0.60
1:A:587:LYS:H	1:A:587:LYS:CD	2.15	0.60
3:C:396:ILE:H	3:C:396:ILE:HD13	1.66	0.60
1:A:183:ILE:CG2	1:A:221:LEU:CD2	2.79	0.60
1:A:602:PHE:CD2	1:A:656:PHE:HB2	2.35	0.60
3:C:573:SER:OG	3:C:575:GLU:HB2	2.01	0.60
1:A:700:ILE:CD1	1:A:719:LEU:CD2	2.74	0.60
1:A:51:ARG:H	1:A:52:PRO:HD2	1.67	0.60
1:A:589:PHE:CD1	1:A:669:ILE:HD11	2.37	0.60
1:A:233:LEU:O	1:A:234:LYS:C	2.39	0.59
3:C:889:ARG:HG3	3:C:904:ASN:HD21	1.67	0.59
3:C:407:ILE:HG21	3:C:410:LEU:HD23	1.84	0.59
1:A:707:ARG:O	1:A:708:LYS:C	2.40	0.59
1:A:751:ASN:HD22	1:A:751:ASN:N	2.00	0.59
3:C:498:ILE:N	3:C:498:ILE:HD12	2.17	0.59
1:A:138:CYS:SG	1:A:182:ILE:HD11	2.42	0.59
1:A:725:PHE:HB2	1:A:726:PRO:HD2	1.84	0.59
3:C:441:GLU:O	3:C:441:GLU:HG2	2.02	0.59
1:A:192:THR:O	1:A:196:ILE:HG13	2.02	0.59
1:A:417:LEU:HD23	1:A:460:ARG:HH12	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ILE:HD12	1:A:521:ILE:N	2.18	0.59
3:C:922:LEU:HD23	3:C:957:VAL:HG13	1.85	0.59
4:D:110:TYR:CZ	4:D:114:LEU:HD11	2.37	0.59
1:A:118:ILE:CD1	1:A:181:HIS:CB	2.44	0.59
3:C:414:ARG:HB3	3:C:462:ASN:HD21	1.68	0.59
1:A:454:LYS:HD2	1:A:534:PRO:HG3	1.83	0.59
3:C:673:LEU:HD23	3:C:674:LYS:H	1.68	0.59
1:A:699:ALA:HB1	1:A:722:GLN:HE22	1.64	0.59
1:A:282:THR:O	1:A:285:PRO:HD2	2.01	0.59
1:A:405:PRO:O	1:A:409:ILE:HG12	2.02	0.59
1:A:296:GLY:O	1:A:297:GLU:CB	2.50	0.59
3:C:692:ALA:C	3:C:693:LEU:HD23	2.23	0.59
1:A:621:ASP:O	1:A:625:ARG:HG2	2.03	0.58
3:C:705:ASP:O	3:C:706:GLU:CB	2.51	0.58
1:A:305:LYS:O	1:A:305:LYS:HG3	2.02	0.58
3:C:851:PHE:HB3	3:C:858:LEU:HD22	1.85	0.58
1:A:692:ARG:HB3	1:A:725:PHE:CD2	2.38	0.58
1:A:228:LYS:HA	1:A:232:GLU:HB2	1.84	0.58
3:C:588:PRO:HB3	3:C:604:CYS:SG	2.43	0.58
1:A:665:PHE:O	1:A:666:ARG:HB2	2.03	0.58
1:A:228:LYS:CE	1:A:232:GLU:HG2	2.34	0.58
3:C:695:ASN:OD1	3:C:697:SER:N	2.30	0.58
1:A:643:PRO:HD2	1:A:652:ASP:HA	1.86	0.58
1:A:601:MET:HB3	1:A:608:PHE:HE2	1.69	0.58
1:A:705:LYS:O	1:A:708:LYS:CE	2.51	0.58
3:C:553:SER:O	3:C:571:LEU:HD12	2.03	0.58
1:A:239:THR:O	1:A:241:CYS:N	2.36	0.58
6:F:5:DT:H73	6:F:6:DA:C6	2.39	0.58
1:A:244:ALA:HA	1:A:293:GLN:OE1	2.03	0.58
3:C:903:CYS:HB3	3:C:942:PHE:CE2	2.39	0.58
1:A:43:LEU:HD12	3:C:402:ILE:HD13	1.85	0.58
1:A:708:LYS:HD3	1:A:708:LYS:N	2.19	0.58
1:A:369:LYS:HE2	1:A:390:MET:CE	2.33	0.58
3:C:704:ILE:H	3:C:704:ILE:HD12	1.68	0.58
1:A:228:LYS:HE2	1:A:232:GLU:OE2	2.03	0.58
3:C:429:PHE:O	3:C:430:VAL:O	2.22	0.58
1:A:240:ASN:ND2	1:A:289:CYS:SG	2.77	0.57
1:A:95:SER:O	1:A:96:HIS:C	2.42	0.57
1:A:540:GLU:CD	1:A:540:GLU:H	2.08	0.57
3:C:712:ILE:O	3:C:712:ILE:HG22	2.03	0.57
1:A:249:ARG:CB	1:A:249:ARG:HH11	2.16	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ASN:HD21	1:A:659:GLU:CB	2.10	0.57
1:A:429:LEU:O	1:A:433:LEU:HB2	2.03	0.57
1:A:528:LEU:HD22	1:A:533:TRP:CZ2	2.40	0.57
3:C:432:GLN:HA	3:C:455:GLN:O	2.04	0.57
3:C:669:SER:O	3:C:670:ASN:C	2.43	0.57
3:C:188:ARG:O	3:C:189:HIS:CG	2.58	0.57
3:C:414:ARG:HG2	3:C:414:ARG:HH11	1.69	0.57
3:C:600:HIS:HB2	3:C:616:LEU:O	2.04	0.57
1:A:468:SER:HB3	1:A:471:ALA:HB2	1.86	0.57
1:A:159:THR:HG22	1:A:160:TYR:N	2.19	0.57
4:D:242:CYS:O	4:D:254:THR:HG23	2.05	0.57
3:C:536:HIS:HB2	3:C:560:LEU:HD13	1.87	0.57
3:C:711:HIS:NE2	3:C:713:ARG:N	2.53	0.57
1:A:541:VAL:HG12	1:A:618:GLY:O	2.05	0.57
3:C:493:PRO:HB2	3:C:494:GLN:HE22	1.70	0.57
1:A:601:MET:CE	1:A:616:ALA:HB2	2.34	0.57
3:C:890:LEU:HB3	3:C:903:CYS:HB2	1.84	0.57
1:A:197:LEU:HB3	1:A:238:GLU:OE1	2.04	0.57
3:C:578:HIS:CE1	3:C:623:LEU:HD12	2.39	0.56
3:C:477:ARG:HG2	3:C:489:GLU:HG3	1.86	0.56
3:C:185:PRO:HG3	4:D:289:ARG:CB	2.30	0.56
3:C:562:THR:C	3:C:564:ILE:H	2.08	0.56
1:A:422:LYS:NZ	1:A:422:LYS:CB	2.59	0.56
1:A:199:LEU:HD13	1:A:209:VAL:CB	2.35	0.56
3:C:454:ASP:N	3:C:454:ASP:OD1	2.28	0.56
1:A:390:MET:O	1:A:390:MET:HE2	2.05	0.56
1:A:390:MET:O	1:A:394:PHE:HB2	2.06	0.56
1:A:84:GLU:HG2	3:C:499:SER:HB3	1.87	0.56
3:C:433:THR:HG22	3:C:434:ARG:H	1.68	0.56
1:A:49:ARG:CD	1:A:51:ARG:HH21	2.18	0.56
3:C:389:ILE:HB	3:C:713:ARG:HB3	1.87	0.56
3:C:165:ILE:CD1	3:C:188:ARG:HH22	2.19	0.56
3:C:502:SER:O	3:C:503:CYS:HB2	2.04	0.56
1:A:129:VAL:CG1	1:A:130:LEU:HG	2.35	0.56
3:C:503:CYS:SG	3:C:504:ASN:N	2.78	0.56
3:C:430:VAL:HG12	3:C:431:GLY:N	2.19	0.56
3:C:403:ASP:HA	3:C:698:THR:HG22	1.88	0.56
1:A:676:GLU:HA	1:A:680:GLU:OE1	2.06	0.56
3:C:644:LEU:HD12	3:C:706:GLU:OE2	2.06	0.56
1:A:751:ASN:C	1:A:753:ASN:H	2.10	0.56
1:A:166:THR:O	1:A:168:PRO:HD3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:HIS:HB2	4:D:453:ASN:HB2	1.88	0.55
1:A:183:ILE:HG23	1:A:221:LEU:HD21	1.88	0.55
1:A:643:PRO:HG2	1:A:652:ASP:HA	1.88	0.55
1:A:155:PHE:O	1:A:159:THR:HB	2.06	0.55
3:C:522:HIS:HB3	3:C:523:PRO:HD2	1.88	0.55
1:A:93:LEU:HD23	1:A:93:LEU:O	2.05	0.55
1:A:601:MET:HE3	1:A:616:ALA:CB	2.36	0.55
3:C:525:GLU:OE2	3:C:527:ARG:NH2	2.39	0.55
3:C:479:VAL:HG12	3:C:480:SER:N	2.22	0.55
3:C:433:THR:HG22	3:C:434:ARG:N	2.22	0.55
1:A:197:LEU:HD21	1:A:235:PHE:CA	2.37	0.55
3:C:493:PRO:HB2	3:C:494:GLN:NE2	2.21	0.55
1:A:129:VAL:HG13	1:A:130:LEU:HG	1.89	0.55
1:A:72:ALA:HB3	1:A:79:ILE:HG23	1.88	0.55
3:C:481:GLN:HA	3:C:484:LYS:HZ3	1.71	0.55
1:A:227:TYR:HD1	1:A:228:LYS:N	2.04	0.55
1:A:570:GLN:CG	2:B:32:LEU:HD11	2.37	0.55
3:C:659:ILE:HG22	3:C:660:TYR:N	2.22	0.55
3:C:502:SER:OG	3:C:543:ILE:HG12	2.07	0.55
1:A:292:LYS:HG3	1:A:330:ARG:NH2	2.22	0.55
1:A:421:ASN:O	1:A:424:ALA:HB2	2.07	0.55
3:C:582:LEU:CD1	3:C:583:GLY:H	2.19	0.55
1:A:267:LEU:HD23	1:A:290:VAL:HG11	1.87	0.55
1:A:448:VAL:O	1:A:452:PHE:HD1	1.90	0.55
3:C:1000:LEU:HD13	3:C:1002:GLU:HB2	1.88	0.55
3:C:649:VAL:CG1	3:C:650:PHE:H	2.17	0.54
1:A:472:GLU:HG2	1:A:495:PHE:HZ	1.72	0.54
3:C:644:LEU:CD1	3:C:706:GLU:OE2	2.55	0.54
3:C:671:VAL:O	3:C:673:LEU:N	2.38	0.54
3:C:431:GLY:O	3:C:432:GLN:HB3	2.07	0.54
1:A:171:TRP:CZ3	1:A:175:LEU:HD11	2.42	0.54
1:A:699:ALA:CB	1:A:722:GLN:HE21	2.17	0.54
3:C:448:LEU:HD23	3:C:451:PHE:CE2	2.42	0.54
3:C:532:THR:OG1	3:C:574:PHE:HD2	1.91	0.54
1:A:733:LYS:O	1:A:737:GLU:HG3	2.07	0.54
1:A:107:ARG:HH12	1:A:173:MET:HG3	1.63	0.54
1:A:597:LEU:O	1:A:598:VAL:C	2.45	0.54
1:A:81:TYR:O	1:A:82:ASN:ND2	2.41	0.54
3:C:596:PHE:CZ	3:C:649:VAL:HG23	2.43	0.54
3:C:83:LYS:HB3	3:C:1072:PHE:CE2	2.42	0.54
3:C:285:LEU:HB3	3:C:297:LEU:HD11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:579:LYS:HG2	3:C:581:MET:HE3	1.89	0.54
1:A:708:LYS:HD3	1:A:708:LYS:H	1.72	0.54
3:C:602:LEU:O	3:C:603:LEU:HD23	2.07	0.54
1:A:630:SER:OG	1:A:672:ILE:HD11	2.07	0.54
3:C:532:THR:CG2	3:C:533:GLU:N	2.69	0.54
3:C:518:TYR:CD1	3:C:518:TYR:C	2.79	0.54
1:A:655:ILE:HD12	1:A:655:ILE:N	2.23	0.54
3:C:518:TYR:CD1	3:C:519:LEU:N	2.75	0.54
3:C:931:LEU:HD21	3:C:944:GLU:HG3	1.90	0.54
1:A:628:LEU:O	1:A:630:SER:O	2.26	0.53
1:A:65:LYS:HD2	1:A:81:TYR:CD2	2.43	0.53
1:A:84:GLU:O	1:A:87:TYR:HB3	2.08	0.53
4:D:124:GLN:HG3	4:D:124:GLN:O	2.08	0.53
1:A:287:ILE:O	1:A:291:GLU:HG3	2.07	0.53
3:C:562:THR:C	3:C:564:ILE:N	2.60	0.53
1:A:316:VAL:CB	1:A:317:PRO:HD3	2.38	0.53
1:A:182:ILE:HG22	1:A:183:ILE:HG13	1.89	0.53
3:C:184:ASP:HB2	3:C:185:PRO:CD	2.38	0.53
1:A:347:PHE:CE1	1:A:351:ILE:HD11	2.43	0.53
1:A:267:LEU:HD13	1:A:328:ARG:NH1	2.22	0.53
3:C:614:PHE:N	3:C:614:PHE:CD1	2.75	0.53
1:A:82:ASN:HD21	1:A:85:GLU:CD	2.12	0.53
6:F:5:DT:H73	6:F:6:DA:N6	2.24	0.53
4:D:299:VAL:HA	4:D:326:PRO:HB3	1.89	0.53
1:A:406:ALA:HB2	1:A:443:ILE:HG21	1.91	0.53
1:A:468:SER:HB3	1:A:471:ALA:CB	2.39	0.53
1:A:228:LYS:NZ	1:A:232:GLU:HG2	2.24	0.53
1:A:100:PRO:O	1:A:104:LYS:HG3	2.09	0.53
1:A:731:ASP:O	1:A:734:LYS:HB3	2.09	0.53
1:A:676:GLU:O	1:A:676:GLU:HG3	2.09	0.52
1:A:239:THR:C	1:A:241:CYS:N	2.60	0.52
1:A:227:TYR:O	1:A:229:ASP:N	2.37	0.52
1:A:732:LEU:O	1:A:733:LYS:C	2.45	0.52
3:C:289:GLU:HA	3:C:295:VAL:HA	1.89	0.52
3:C:622:LEU:C	3:C:622:LEU:HD12	2.29	0.52
1:A:43:LEU:HD11	3:C:400:ALA:CB	2.12	0.52
1:A:642:SER:C	1:A:644:LYS:H	2.11	0.52
1:A:204:ARG:CZ	1:A:243:TYR:CE2	2.91	0.52
1:A:544:THR:O	1:A:547:MET:HB2	2.08	0.52
2:B:37:ILE:HG12	2:B:38:VAL:N	2.00	0.52
1:A:227:TYR:C	1:A:227:TYR:CD1	2.83	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:525:GLU:OE2	3:C:527:ARG:NE	2.41	0.52
1:A:709:THR:HG22	1:A:710:LEU:N	2.25	0.52
3:C:649:VAL:CG1	3:C:650:PHE:N	2.71	0.52
3:C:658:VAL:HG12	3:C:658:VAL:O	2.09	0.52
1:A:587:LYS:HE3	1:A:664:LEU:O	2.10	0.52
1:A:735:ARG:NE	1:A:735:ARG:HA	2.24	0.52
4:D:119:HIS:O	4:D:121:GLN:N	2.43	0.52
1:A:352:VAL:HG12	1:A:361:MET:SD	2.50	0.52
1:A:625:ARG:O	1:A:629:GLN:N	2.43	0.52
1:A:99:SER:HB2	1:A:100:PRO:CD	2.35	0.52
3:C:659:ILE:HD12	3:C:659:ILE:H	1.75	0.52
1:A:120:PRO:O	1:A:123:GLU:HG3	2.10	0.52
3:C:450:GLY:HA3	3:C:479:VAL:HG22	1.91	0.52
1:A:660:PHE:C	1:A:662:HIS:H	2.14	0.52
3:C:487:VAL:O	3:C:488:SER:HB2	2.09	0.52
3:C:402:ILE:O	3:C:698:THR:HB	2.10	0.52
1:A:643:PRO:CG	1:A:652:ASP:HA	2.39	0.52
3:C:218:MET:CE	3:C:261:HIS:HD2	2.22	0.52
1:A:699:ALA:HB1	1:A:722:GLN:HE21	1.61	0.52
1:A:43:LEU:CD1	3:C:402:ILE:HD13	2.40	0.52
1:A:657:ASN:ND2	1:A:659:GLU:HB2	2.11	0.52
3:C:448:LEU:HD23	3:C:451:PHE:HE2	1.75	0.51
3:C:573:SER:O	3:C:574:PHE:HB2	2.10	0.51
1:A:299:LEU:HD23	1:A:326:PHE:CE2	2.45	0.51
1:A:257:PRO:HB3	1:A:318:ASP:OD1	2.10	0.51
1:A:609:SER:H	1:A:612:GLU:CG	2.24	0.51
3:C:578:HIS:CE1	3:C:623:LEU:CD1	2.94	0.51
4:D:217:THR:OG1	4:D:254:THR:HG21	2.09	0.51
3:C:408:LYS:HA	3:C:678:TYR:CE1	2.46	0.51
1:A:516:SER:O	1:A:517:ASP:O	2.29	0.51
3:C:594:THR:CG2	3:C:595:THR:N	2.73	0.51
3:C:711:HIS:CE1	3:C:712:ILE:C	2.84	0.51
3:C:490:TRP:CG	3:C:491:LYS:N	2.79	0.51
1:A:539:MET:HE3	1:A:619:ILE:HA	1.91	0.51
1:A:404:LYS:O	1:A:405:PRO:C	2.49	0.51
1:A:55:PRO:O	1:A:56:ASP:HB2	2.11	0.51
3:C:416:ASP:OD1	3:C:418:ASN:HB2	2.11	0.51
1:A:158:ARG:NH1	3:C:633:THR:O	2.44	0.51
1:A:583:LYS:O	1:A:584:GLU:HB2	2.10	0.51
1:A:107:ARG:HH11	1:A:173:MET:HG3	1.72	0.51
1:A:757:TYR:HD1	1:A:758:VAL:N	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:471:ILE:HA	3:C:476:VAL:HA	1.92	0.51
1:A:439:LEU:O	1:A:440:PHE:C	2.49	0.51
1:A:183:ILE:HD13	1:A:221:LEU:CD2	2.41	0.51
3:C:459:PHE:CD2	3:C:460:CYS:N	2.79	0.51
3:C:105:HIS:CD2	3:C:1067:LYS:HB2	2.46	0.51
1:A:501:SER:O	1:A:505:MET:HB2	2.11	0.51
3:C:561:TRP:HA	3:C:587:ILE:HG21	1.92	0.50
1:A:228:LYS:CD	1:A:232:GLU:HG2	2.41	0.50
1:A:119:LEU:HB2	1:A:120:PRO:CD	2.37	0.50
1:A:417:LEU:HD23	1:A:460:ARG:NH1	2.26	0.50
3:C:184:ASP:OD1	3:C:184:ASP:C	2.48	0.50
1:A:131:PHE:CD1	1:A:191:LYS:CE	2.95	0.50
1:A:602:PHE:N	1:A:602:PHE:CD1	2.79	0.50
3:C:512:VAL:HB	3:C:515:ALA:HB3	1.94	0.50
1:A:186:LYS:CB	1:A:188:VAL:HG23	2.40	0.50
3:C:570:LYS:O	3:C:574:PHE:N	2.41	0.50
1:A:45:ILE:HD11	3:C:404:LEU:HD21	1.92	0.50
3:C:613:TYR:CE1	3:C:627:LYS:HB2	2.47	0.50
1:A:207:GLU:O	1:A:208:ALA:O	2.30	0.50
1:A:96:HIS:O	1:A:97:LYS:HB2	2.11	0.50
3:C:183:GLN:HA	3:C:188:ARG:HA	1.94	0.50
3:C:663:ASN:HD21	3:C:1131:LYS:HB3	1.76	0.50
1:A:380:PHE:CD2	1:A:386:PHE:CD2	3.00	0.50
1:A:705:LYS:HA	1:A:757:TYR:CE2	2.43	0.50
1:A:135:ILE:CD1	1:A:188:VAL:HG12	2.30	0.50
1:A:182:ILE:O	1:A:188:VAL:HG11	2.12	0.50
3:C:451:PHE:HD1	3:C:470:GLN:HB2	1.74	0.50
1:A:587:LYS:HD2	1:A:587:LYS:N	2.25	0.50
1:A:141:ASP:C	1:A:143:CYS:N	2.64	0.49
1:A:173:MET:HG2	1:A:173:MET:O	2.11	0.49
3:C:492:GLU:CG	3:C:496:LYS:HB2	2.42	0.49
1:A:74:GLN:O	1:A:75:SER:C	2.49	0.49
1:A:206:GLY:O	1:A:207:GLU:O	2.30	0.49
1:A:757:TYR:CE1	1:A:759:ALA:HA	2.37	0.49
1:A:601:MET:HE1	1:A:616:ALA:HB2	1.91	0.49
3:C:893:TRP:HE3	3:C:899:LEU:HD13	1.77	0.49
1:A:382:LYS:O	1:A:383:ASN:C	2.50	0.49
1:A:707:ARG:O	1:A:709:THR:O	2.30	0.49
1:A:710:LEU:O	1:A:711:GLY:O	2.30	0.49
3:C:668:PHE:CD1	3:C:668:PHE:N	2.80	0.49
4:D:211:SER:HB3	4:D:243:VAL:HG13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:612:PHE:CE2	3:C:628:LYS:HD2	2.47	0.49
3:C:514:ARG:HG3	3:C:514:ARG:HH11	1.78	0.49
3:C:715:VAL:O	3:C:715:VAL:HG12	2.12	0.49
3:C:1054:MET:SD	3:C:1129:LEU:HD11	2.52	0.49
1:A:82:ASN:OD1	1:A:82:ASN:O	2.30	0.49
1:A:330:ARG:H	1:A:330:ARG:CD	2.26	0.49
3:C:704:ILE:O	3:C:705:ASP:CB	2.57	0.49
1:A:412:HIS:HE1	1:A:416:LYS:HE3	1.77	0.49
3:C:596:PHE:CE2	3:C:659:ILE:HG22	2.48	0.49
3:C:709:LYS:O	3:C:710:LEU:O	2.30	0.49
1:A:347:PHE:O	1:A:351:ILE:HG13	2.12	0.49
4:D:256:ASP:OD2	4:D:260:ARG:HB2	2.13	0.49
3:C:596:PHE:HZ	3:C:649:VAL:HG23	1.78	0.49
1:A:457:LEU:HD22	1:A:461:LEU:HD12	1.94	0.49
3:C:594:THR:HG23	3:C:595:THR:N	2.28	0.49
4:D:111:LYS:HE2	4:D:118:ILE:CB	2.43	0.49
1:A:696:ILE:CD1	1:A:725:PHE:CZ	2.93	0.49
1:A:203:GLU:O	1:A:205:SER:N	2.45	0.49
3:C:490:TRP:CD2	3:C:491:LYS:N	2.81	0.49
1:A:469:VAL:HG12	1:A:473:LYS:HE3	1.94	0.49
1:A:197:LEU:CD2	1:A:235:PHE:CA	2.80	0.49
3:C:578:HIS:HD2	3:C:623:LEU:H	1.55	0.49
2:B:21:ARG:O	2:B:22:PHE:CD1	2.66	0.49
1:A:440:PHE:CE2	1:A:446:LYS:HD3	2.47	0.49
1:A:726:PRO:O	1:A:727:VAL:CB	2.60	0.49
1:A:49:ARG:CD	1:A:51:ARG:NH2	2.75	0.49
1:A:124:ASP:N	1:A:124:ASP:OD1	2.46	0.49
1:A:649:GLU:HB2	1:A:652:ASP:OD2	2.13	0.48
3:C:731:GLN:HA	3:C:796:GLN:HE21	1.78	0.48
3:C:587:ILE:HD12	3:C:587:ILE:H	1.78	0.48
1:A:57:ASN:C	1:A:59:THR:H	2.14	0.48
1:A:601:MET:HE1	1:A:613:ILE:HA	1.95	0.48
4:D:272:PHE:HE2	4:D:312:LYS:HA	1.78	0.48
1:A:751:ASN:ND2	1:A:751:ASN:O	2.46	0.48
1:A:300:THR:O	1:A:304:GLN:HB2	2.13	0.48
3:C:770:LEU:HD13	3:C:865:GLU:HB2	1.96	0.48
3:C:571:LEU:O	3:C:572:PRO:C	2.50	0.48
1:A:63:TRP:HH2	1:A:102:LEU:CA	2.25	0.48
3:C:641:PHE:CE2	3:C:650:PHE:HB2	2.48	0.48
3:C:182:TYR:O	3:C:188:ARG:CA	2.61	0.48
1:A:92:ASN:ND2	3:C:408:LYS:NZ	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CE2	1:A:188:VAL:CG1	2.91	0.48
2:B:38:VAL:O	2:B:39:VAL:O	2.30	0.48
1:A:197:LEU:HD11	1:A:234:LYS:HB3	1.94	0.48
1:A:82:ASN:O	1:A:83:LEU:O	2.31	0.48
1:A:457:LEU:O	1:A:460:ARG:N	2.47	0.48
3:C:565:SER:OG	3:C:567:ARG:NH1	2.46	0.48
3:C:659:ILE:O	3:C:660:TYR:HB3	2.14	0.48
3:C:641:PHE:HB2	3:C:681:PRO:HG3	1.94	0.48
1:A:206:GLY:O	1:A:207:GLU:C	2.51	0.48
3:C:602:LEU:HD13	3:C:602:LEU:C	2.33	0.48
3:C:1136:LEU:O	3:C:1139:ILE:HG12	2.13	0.48
1:A:541:VAL:HG23	1:A:543:LEU:CD2	2.43	0.48
3:C:443:VAL:HG12	3:C:443:VAL:O	2.13	0.48
1:A:515:GLN:O	1:A:515:GLN:HG2	2.14	0.48
1:A:315:ARG:O	1:A:319:LEU:HG	2.14	0.48
3:C:1109:VAL:O	3:C:1111:ASN:N	2.42	0.48
1:A:624:LEU:HD22	1:A:628:LEU:CD1	2.44	0.48
3:C:457:THR:HG22	3:C:458:PHE:N	2.29	0.48
1:A:751:ASN:ND2	1:A:751:ASN:N	2.61	0.48
3:C:218:MET:HE2	3:C:261:HIS:HD2	1.79	0.48
1:A:692:ARG:HB3	1:A:725:PHE:HE2	1.69	0.48
1:A:719:LEU:HD22	1:A:723:LEU:HD21	1.96	0.48
1:A:82:ASN:O	1:A:82:ASN:CG	2.53	0.48
1:A:401:ARG:NH2	1:A:404:LYS:HG3	2.29	0.48
1:A:448:VAL:O	1:A:451:ALA:HB3	2.14	0.48
1:A:106:LEU:HD22	1:A:153:PHE:CD2	2.49	0.47
1:A:629:GLN:O	1:A:633:CYS:HB2	2.14	0.47
1:A:529:THR:HA	2:B:33:TRP:CD1	2.49	0.47
3:C:184:ASP:O	3:C:185:PRO:C	2.50	0.47
3:C:459:PHE:O	3:C:460:CYS:HB3	2.13	0.47
3:C:479:VAL:CG1	3:C:480:SER:N	2.77	0.47
1:A:450:GLU:OE2	1:A:454:LYS:HE3	2.14	0.47
1:A:544:THR:HG23	1:A:545:PRO:HD2	1.96	0.47
4:D:394:PRO:HB3	4:D:402:ASP:HB3	1.96	0.47
1:A:70:VAL:HG21	1:A:106:LEU:HD13	1.95	0.47
1:A:73:VAL:C	1:A:74:GLN:O	2.45	0.47
1:A:248:GLN:O	1:A:249:ARG:C	2.52	0.47
1:A:748:ASP:C	1:A:750:ASP:H	2.17	0.47
3:C:459:PHE:CG	3:C:460:CYS:N	2.82	0.47
3:C:587:ILE:HD12	3:C:587:ILE:N	2.29	0.47
1:A:417:LEU:CD2	1:A:460:ARG:HH12	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:MET:HE3	1:A:251:MET:HA	1.97	0.47
3:C:679:MET:SD	3:C:679:MET:C	2.93	0.47
3:C:450:GLY:O	3:C:477:ARG:NH2	2.46	0.47
1:A:588:GLU:O	1:A:666:ARG:HA	2.15	0.47
3:C:1048:TYR:O	3:C:1052:LEU:HB2	2.15	0.47
1:A:341:SER:HB3	1:A:389:LEU:HD12	1.97	0.47
1:A:74:GLN:HA	1:A:145:GLN:NE2	2.30	0.47
1:A:170:ILE:O	1:A:173:MET:HB3	2.14	0.47
1:A:627:THR:O	1:A:631:LEU:HD23	2.14	0.47
1:A:196:ILE:HG21	1:A:231:PHE:CE1	2.50	0.47
3:C:189:HIS:CD2	3:C:189:HIS:N	2.83	0.47
1:A:241:CYS:O	1:A:244:ALA:HB3	2.15	0.47
3:C:657:THR:HG22	3:C:658:VAL:N	2.25	0.47
1:A:308:ASP:OD1	1:A:343:TYR:HD2	1.97	0.47
3:C:433:THR:O	3:C:434:ARG:HG3	2.14	0.47
3:C:663:ASN:HD21	3:C:1131:LYS:CB	2.27	0.47
1:A:641:LYS:HE2	1:A:647:GLU:O	2.14	0.47
1:A:707:ARG:HD3	1:A:710:LEU:HD13	1.96	0.47
1:A:437:MET:HE3	1:A:478:LYS:HD2	1.96	0.47
1:A:482:GLU:O	1:A:483:CYS:HB2	2.14	0.47
3:C:579:LYS:HE3	3:C:581:MET:CE	2.45	0.47
1:A:638:VAL:HG12	1:A:639:LEU:CD2	2.31	0.47
1:A:660:PHE:C	1:A:662:HIS:N	2.67	0.47
1:A:95:SER:O	1:A:96:HIS:O	2.33	0.47
3:C:385:GLY:HA3	3:C:719:GLU:O	2.14	0.47
3:C:403:ASP:O	3:C:405:PRO:HD3	2.15	0.47
1:A:757:TYR:CD1	1:A:758:VAL:N	2.82	0.47
3:C:43:VAL:HG21	3:C:50:ARG:CZ	2.45	0.47
1:A:263:VAL:HG11	1:A:295:LEU:HD21	1.97	0.46
3:C:643:SER:OG	3:C:644:LEU:N	2.47	0.46
3:C:438:LEU:CD1	3:C:684:SER:HB2	2.46	0.46
3:C:638:LEU:O	3:C:639:ARG:HG2	2.15	0.46
1:A:696:ILE:CG1	1:A:725:PHE:HZ	2.28	0.46
1:A:592:SER:HB2	1:A:673:GLN:NE2	2.29	0.46
3:C:1055:GLN:NE2	3:C:1090:ASP:H	2.09	0.46
3:C:704:ILE:N	3:C:704:ILE:HD12	2.30	0.46
3:C:531:HIS:ND1	3:C:532:THR:N	2.63	0.46
1:A:732:LEU:O	1:A:735:ARG:N	2.45	0.46
3:C:407:ILE:CD1	3:C:699:LEU:HB2	2.44	0.46
1:A:196:ILE:HD13	1:A:218:LEU:HD23	1.93	0.46
1:A:204:ARG:NE	1:A:243:TYR:OH	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:ILE:O	3:C:396:ILE:HD13	2.15	0.46
3:C:596:PHE:CZ	3:C:659:ILE:HG22	2.50	0.46
3:C:402:ILE:HG22	3:C:403:ASP:H	1.80	0.46
1:A:630:SER:C	1:A:632:ALA:N	2.67	0.46
1:A:321:GLN:O	1:A:325:LEU:HD12	2.16	0.46
3:C:656:PRO:HG2	3:C:676:VAL:HG23	1.97	0.46
1:A:83:LEU:O	1:A:85:GLU:N	2.49	0.46
3:C:695:ASN:OD1	3:C:698:THR:N	2.41	0.46
1:A:705:LYS:HD3	1:A:705:LYS:C	2.35	0.46
1:A:200:ILE:O	1:A:203:GLU:N	2.25	0.46
3:C:414:ARG:HB3	3:C:462:ASN:ND2	2.29	0.46
1:A:440:PHE:CZ	1:A:446:LYS:HD3	2.51	0.46
1:A:303:LEU:HD23	1:A:322:MET:CE	2.46	0.46
3:C:312:GLU:HG3	3:C:327:ARG:HD2	1.98	0.46
1:A:113:HIS:O	1:A:117:GLN:HG2	2.16	0.46
3:C:23:PHE:N	3:C:30:ASN:ND2	2.59	0.46
1:A:534:PRO:HB2	1:A:536:TYR:CE1	2.51	0.46
3:C:953:TRP:HB2	3:C:970:ASN:HB2	1.98	0.46
1:A:130:LEU:O	1:A:131:PHE:C	2.54	0.46
1:A:131:PHE:CZ	1:A:188:VAL:HG22	2.51	0.46
1:A:587:LYS:HD3	1:A:660:PHE:CE2	2.51	0.46
3:C:889:ARG:HD2	3:C:891:TYR:CZ	2.51	0.46
3:C:407:ILE:HD11	3:C:699:LEU:HB2	1.98	0.46
3:C:512:VAL:O	3:C:515:ALA:HB3	2.15	0.46
3:C:442:GLU:HG3	3:C:443:VAL:H	1.81	0.46
1:A:375:VAL:HG13	1:A:379:CYS:HB2	1.98	0.46
1:A:491:LEU:HA	1:A:494:MET:CG	2.33	0.45
1:A:92:ASN:ND2	3:C:408:LYS:HZ1	2.14	0.45
6:F:5:DT:C7	6:F:6:DA:C6	2.99	0.45
1:A:193:ILE:C	1:A:195:GLY:N	2.68	0.45
1:A:632:ALA:O	1:A:633:CYS:C	2.55	0.45
3:C:490:TRP:O	3:C:491:LYS:HB2	2.15	0.45
1:A:587:LYS:HB2	1:A:660:PHE:CE2	2.51	0.45
3:C:705:ASP:O	3:C:706:GLU:HB3	2.16	0.45
1:A:267:LEU:CD2	1:A:290:VAL:HG11	2.46	0.45
3:C:869:ALA:H	3:C:885:ASN:ND2	2.14	0.45
1:A:179:ARG:O	1:A:184:SER:HB3	2.16	0.45
1:A:202:ARG:HH21	1:A:207:GLU:CD	2.19	0.45
3:C:411:TRP:HB2	3:C:460:CYS:SG	2.56	0.45
1:A:433:LEU:HD23	1:A:478:LYS:HE3	1.97	0.45
1:A:601:MET:CE	1:A:616:ALA:HB3	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:ILE:CD1	3:C:396:ILE:N	2.79	0.45
1:A:341:SER:CB	1:A:389:LEU:HD12	2.46	0.45
1:A:527:ILE:CG2	1:A:527:ILE:O	2.65	0.45
4:D:122:LEU:O	4:D:123:ARG:C	2.54	0.45
1:A:55:PRO:O	1:A:56:ASP:CB	2.64	0.45
1:A:303:LEU:HD13	1:A:339:HIS:CD2	2.52	0.45
2:B:20:LYS:HB2	2:B:20:LYS:HE3	1.72	0.45
2:B:38:VAL:O	2:B:39:VAL:C	2.55	0.45
1:A:704:MET:O	1:A:757:TYR:HD2	2.00	0.45
1:A:100:PRO:HG3	1:A:160:TYR:CZ	2.51	0.45
1:A:196:ILE:HG21	1:A:218:LEU:HD21	1.99	0.45
3:C:312:GLU:HG3	3:C:327:ARG:CD	2.47	0.45
2:B:37:ILE:H	2:B:37:ILE:HD12	1.82	0.45
3:C:659:ILE:CG2	3:C:660:TYR:N	2.80	0.45
1:A:292:LYS:O	1:A:293:GLN:HG2	2.17	0.45
1:A:295:LEU:HD11	1:A:325:LEU:HD22	1.99	0.45
4:D:123:ARG:HA	4:D:126:LEU:HD12	1.97	0.45
1:A:271:GLY:C	1:A:273:ARG:H	2.20	0.45
3:C:921:ILE:HB	3:C:933:LEU:HB2	1.99	0.45
3:C:663:ASN:HD21	3:C:1131:LYS:HG2	1.81	0.45
1:A:114:VAL:O	1:A:117:GLN:N	2.50	0.45
1:A:141:ASP:OD2	1:A:144:ARG:NH2	2.46	0.45
1:A:200:ILE:O	1:A:202:ARG:N	2.50	0.45
1:A:203:GLU:C	1:A:205:SER:N	2.70	0.45
1:A:580:ALA:HB2	2:B:22:PHE:HE1	1.82	0.45
1:A:460:ARG:NH1	1:A:472:GLU:OE2	2.49	0.45
1:A:539:MET:HE1	1:A:619:ILE:HG23	1.99	0.45
3:C:926:LEU:HD21	4:D:129:PRO:HG3	1.99	0.45
3:C:478:LEU:HB3	3:C:488:SER:HB3	1.99	0.45
2:B:19:LYS:HA	2:B:19:LYS:CE	2.35	0.45
1:A:437:MET:HE2	1:A:475:MET:HE1	1.99	0.45
1:A:329:VAL:CG1	1:A:330:ARG:H	2.23	0.45
1:A:264:SER:O	1:A:268:GLU:HG2	2.17	0.45
3:C:607:GLY:HA2	3:C:635:PRO:HB3	1.99	0.45
3:C:390:ILE:HG22	3:C:391:ARG:N	2.32	0.45
3:C:597:GLU:O	3:C:598:SER:HB3	2.16	0.45
1:A:710:LEU:O	1:A:711:GLY:C	2.55	0.44
1:A:61:ASP:O	1:A:65:LYS:HG3	2.17	0.44
1:A:93:LEU:CD2	1:A:93:LEU:C	2.82	0.44
1:A:601:MET:HB3	1:A:608:PHE:CE2	2.49	0.44
1:A:668:LYS:NZ	1:A:670:ASN:HB3	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:388:ILE:O	4:D:408:ILE:HA	2.17	0.44
1:A:434:ASP:O	1:A:438:ILE:HG13	2.18	0.44
1:A:70:VAL:O	1:A:72:ALA:N	2.50	0.44
1:A:227:TYR:CD1	1:A:228:LYS:N	2.83	0.44
3:C:707:ILE:HG23	3:C:708:GLN:H	1.80	0.44
1:A:526:ASN:HD22	1:A:526:ASN:HA	1.61	0.44
1:A:183:ILE:CD1	1:A:220:MET:CE	2.75	0.44
1:A:274:VAL:CG1	1:A:283:GLN:HE21	2.23	0.44
3:C:476:VAL:HG22	3:C:526:LEU:CD1	2.47	0.44
3:C:740:ILE:HG23	3:C:785:GLU:HG3	1.99	0.44
3:C:1057:ARG:HH12	3:C:1110:ALA:HB3	1.83	0.44
3:C:580:GLU:OE2	3:C:626:ARG:HD2	2.17	0.44
3:C:451:PHE:HE1	3:C:470:GLN:HB2	1.79	0.44
1:A:610:PHE:CE1	1:A:614:LYS:HE3	2.52	0.44
1:A:349:THR:C	1:A:351:ILE:H	2.21	0.44
1:A:256:VAL:O	1:A:257:PRO:C	2.56	0.44
3:C:546:LEU:O	3:C:549:SER:HB3	2.17	0.44
3:C:528:GLN:HG2	3:C:528:GLN:O	2.16	0.44
1:A:696:ILE:HG12	1:A:725:PHE:HZ	1.81	0.44
3:C:629:VAL:HG23	3:C:630:THR:N	2.31	0.44
3:C:165:ILE:HG13	3:C:188:ARG:NH1	2.33	0.44
3:C:447:GLU:O	3:C:448:LEU:HD12	2.18	0.44
3:C:692:ALA:O	3:C:693:LEU:HD23	2.18	0.44
3:C:586:ILE:HG22	3:C:607:GLY:H	1.83	0.44
1:A:453:TYR:C	1:A:453:TYR:CD1	2.91	0.44
3:C:81:THR:HG21	3:C:85:ASN:ND2	2.22	0.44
1:A:184:SER:O	1:A:186:LYS:N	2.50	0.44
1:A:758:VAL:O	1:A:758:VAL:HG12	2.17	0.44
1:A:90:VAL:O	1:A:92:ASN:N	2.51	0.44
1:A:143:CYS:O	1:A:147:ILE:HG13	2.17	0.44
3:C:641:PHE:HB3	3:C:679:MET:HE1	1.99	0.44
3:C:396:ILE:N	3:C:396:ILE:HD13	2.29	0.44
1:A:251:MET:HE3	1:A:259:TYR:CE1	2.53	0.44
1:A:222:SER:O	1:A:224:LEU:N	2.51	0.44
1:A:70:VAL:CG2	1:A:106:LEU:HD11	2.47	0.43
1:A:65:LYS:HD2	1:A:81:TYR:HD2	1.82	0.43
4:D:382:HIS:CG	4:D:383:PRO:HD2	2.53	0.43
1:A:704:MET:HG3	1:A:745:MET:CE	2.48	0.43
1:A:307:LEU:O	1:A:308:ASP:C	2.56	0.43
1:A:693:GLN:O	1:A:696:ILE:HB	2.18	0.43
3:C:532:THR:CG2	3:C:533:GLU:H	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:430:VAL:O	3:C:456:GLN:HB2	2.18	0.43
1:A:412:HIS:CE1	1:A:416:LYS:HE3	2.53	0.43
1:A:725:PHE:HB2	1:A:726:PRO:CD	2.47	0.43
3:C:582:LEU:CD1	3:C:583:GLY:N	2.81	0.43
1:A:90:VAL:O	1:A:94:CYS:N	2.42	0.43
3:C:429:PHE:O	3:C:456:GLN:HG3	2.18	0.43
3:C:663:ASN:HD21	3:C:1131:LYS:CG	2.30	0.43
3:C:893:TRP:CE3	3:C:899:LEU:HD13	2.54	0.43
3:C:419:ARG:HD3	3:C:421:THR:O	2.18	0.43
3:C:185:PRO:HB2	3:C:186:GLN:NE2	2.33	0.43
1:A:704:MET:O	1:A:757:TYR:HB2	2.18	0.43
1:A:617:THR:OG1	1:A:618:GLY:N	2.50	0.43
1:A:712:HIS:C	1:A:712:HIS:CD2	2.90	0.43
1:A:183:ILE:CG2	1:A:221:LEU:HD21	2.48	0.43
3:C:184:ASP:C	3:C:186:GLN:N	2.72	0.43
1:A:428:GLU:O	1:A:432:THR:HG23	2.18	0.43
5:E:10:DG:C2	6:F:4:DG:C2	3.06	0.43
3:C:428:SER:OG	3:C:456:GLN:HG2	2.18	0.43
1:A:545:PRO:O	1:A:546:GLU:C	2.56	0.43
1:A:193:ILE:C	1:A:195:GLY:H	2.22	0.43
3:C:586:ILE:HG21	3:C:608:ASP:N	2.34	0.43
1:A:149:ILE:O	1:A:150:ARG:C	2.56	0.43
1:A:63:TRP:CH2	1:A:102:LEU:HG	2.53	0.43
1:A:390:MET:HE2	1:A:390:MET:C	2.38	0.43
3:C:532:THR:HG22	3:C:533:GLU:H	1.80	0.43
1:A:523:LEU:HD11	1:A:525:VAL:CG2	2.49	0.43
4:D:279:ALA:HB1	4:D:299:VAL:HG22	2.01	0.43
1:A:440:PHE:O	1:A:442:PHE:N	2.51	0.43
1:A:450:GLU:HG3	1:A:451:ALA:N	2.34	0.43
4:D:383:PRO:HG3	4:D:435:SER:O	2.18	0.43
1:A:279:ASP:O	1:A:281:SER:N	2.52	0.43
1:A:311:LEU:HD11	1:A:340:TRP:HD1	1.84	0.43
3:C:889:ARG:CD	3:C:901:THR:HB	2.45	0.43
3:C:1097:PHE:O	3:C:1100:ILE:HG12	2.19	0.43
1:A:84:GLU:O	1:A:85:GLU:C	2.57	0.42
1:A:555:LYS:HD2	1:A:569:TRP:CZ3	2.47	0.42
3:C:407:ILE:HD13	3:C:699:LEU:HD23	2.01	0.42
1:A:583:LYS:O	1:A:584:GLU:CB	2.66	0.42
1:A:131:PHE:CZ	1:A:188:VAL:CB	2.75	0.42
3:C:565:SER:HB2	3:C:581:MET:HE2	2.01	0.42
3:C:657:THR:CG2	3:C:668:PHE:HB3	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:494:GLN:O	3:C:495:ALA:HB3	2.19	0.42
3:C:505:SER:OG	3:C:506:SER:N	2.51	0.42
4:D:367:PRO:HG2	4:D:392:ARG:HG3	2.01	0.42
1:A:696:ILE:CG1	1:A:725:PHE:CZ	3.01	0.42
1:A:437:MET:O	1:A:440:PHE:HB3	2.19	0.42
3:C:603:LEU:HD23	3:C:603:LEU:N	2.33	0.42
1:A:542:HIS:HB2	1:A:617:THR:HA	2.00	0.42
1:A:592:SER:OG	1:A:595:GLN:HG3	2.19	0.42
1:A:609:SER:O	1:A:610:PHE:C	2.57	0.42
3:C:500:VAL:HG12	3:C:541:LEU:HD12	2.01	0.42
1:A:141:ASP:O	1:A:145:GLN:HG2	2.19	0.42
4:D:323:HIS:CD2	4:D:342:THR:HG21	2.53	0.42
1:A:541:VAL:HG23	1:A:543:LEU:HD21	2.02	0.42
1:A:399:ASN:ND2	1:A:444:HIS:CE1	2.87	0.42
4:D:391:GLY:HA3	4:D:429:ILE:O	2.19	0.42
3:C:611:LEU:HD23	3:C:611:LEU:C	2.40	0.42
1:A:122:ARG:CZ	1:A:186:LYS:HZ1	2.30	0.42
1:A:496:LYS:HA	1:A:496:LYS:HD3	1.84	0.42
5:E:4:DA:C2	6:F:10:DA:C2	3.07	0.42
3:C:1030:PHE:CZ	3:C:1038:GLY:HA3	2.55	0.42
1:A:110:CYS:O	1:A:111:GLU:C	2.58	0.42
1:A:59:THR:O	1:A:63:TRP:HD1	2.02	0.42
3:C:356:LEU:CD2	3:C:712:ILE:HG21	2.49	0.42
1:A:578:LEU:HD13	1:A:591:VAL:HG21	1.99	0.42
1:A:530:MET:HB2	2:B:33:TRP:O	2.19	0.42
1:A:555:LYS:HB2	1:A:569:TRP:HH2	1.84	0.42
3:C:1102:ARG:N	3:C:1103:PRO:HD2	2.35	0.42
1:A:425:THR:HG22	1:A:426:ASP:N	2.35	0.42
1:A:118:ILE:CG1	1:A:181:HIS:CB	2.86	0.42
1:A:182:ILE:CG2	1:A:183:ILE:HG13	2.50	0.42
1:A:72:ALA:HB1	1:A:77:THR:HB	2.01	0.42
3:C:230:ILE:HD11	3:C:285:LEU:HD21	2.02	0.42
1:A:75:SER:O	1:A:77:THR:N	2.53	0.42
1:A:218:LEU:HD12	1:A:277:TYR:HB2	2.00	0.42
1:A:200:ILE:O	1:A:201:GLU:C	2.58	0.42
1:A:437:MET:HE1	1:A:475:MET:HE3	2.02	0.42
4:D:289:ARG:NH2	4:D:335:THR:O	2.53	0.42
1:A:707:ARG:HD3	1:A:710:LEU:HD22	2.02	0.42
3:C:578:HIS:CG	3:C:623:LEU:HD12	2.54	0.42
3:C:404:LEU:HD12	3:C:429:PHE:CZ	2.55	0.42
3:C:576:LEU:C	3:C:577:LEU:HD23	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:563:ASP:OD2	3:C:565:SER:HB3	2.20	0.42
1:A:640:ILE:O	1:A:655:ILE:HD12	2.20	0.42
3:C:185:PRO:HD3	4:D:289:ARG:CB	2.28	0.41
1:A:536:TYR:CD2	1:A:573:LEU:HD11	2.54	0.41
1:A:221:LEU:HA	1:A:221:LEU:HD23	1.91	0.41
3:C:571:LEU:HA	3:C:571:LEU:HD23	1.87	0.41
3:C:708:GLN:HB3	3:C:709:LYS:H	1.60	0.41
1:A:597:LEU:HA	1:A:600:LEU:HD12	2.01	0.41
3:C:404:LEU:HD13	3:C:404:LEU:HA	1.89	0.41
3:C:184:ASP:CB	3:C:185:PRO:CD	2.97	0.41
3:C:185:PRO:CD	4:D:289:ARG:CB	2.78	0.41
3:C:523:PRO:HB3	3:C:524:GLN:NE2	2.35	0.41
3:C:24:THR:H	3:C:30:ASN:ND2	2.18	0.41
1:A:390:MET:HE2	1:A:394:PHE:HB2	2.02	0.41
1:A:267:LEU:HD21	1:A:290:VAL:HG12	2.03	0.41
1:A:189:GLN:CD	1:A:230:SER:HB3	2.41	0.41
1:A:74:GLN:NE2	1:A:110:CYS:HA	2.15	0.41
1:A:744:TYR:O	1:A:757:TYR:O	2.38	0.41
1:A:651:GLY:O	1:A:652:ASP:C	2.57	0.41
1:A:232:GLU:O	1:A:235:PHE:HB3	2.20	0.41
1:A:49:ARG:HA	1:A:49:ARG:NE	2.35	0.41
3:C:602:LEU:HD22	3:C:603:LEU:N	2.34	0.41
3:C:673:LEU:HD23	3:C:674:LYS:N	2.33	0.41
4:D:347:ASN:HA	4:D:366:HIS:O	2.21	0.41
1:A:131:PHE:O	1:A:134:LYS:HB2	2.21	0.41
1:A:79:ILE:H	1:A:79:ILE:CD1	2.23	0.41
3:C:567:ARG:HB3	3:C:579:LYS:HA	2.01	0.41
3:C:711:HIS:CE1	3:C:713:ARG:N	2.88	0.41
1:A:123:GLU:HB3	1:A:124:ASP:H	1.61	0.41
1:A:250:LEU:HD22	1:A:254:ARG:HD3	2.01	0.41
1:A:63:TRP:HZ3	1:A:102:LEU:HA	1.75	0.41
3:C:641:PHE:CD1	3:C:641:PHE:C	2.93	0.41
3:C:182:TYR:O	3:C:188:ARG:HA	2.20	0.41
1:A:184:SER:O	1:A:185:ASP:C	2.58	0.41
1:A:219:GLY:O	1:A:220:MET:C	2.57	0.41
1:A:757:TYR:O	1:A:758:VAL:CB	2.65	0.41
1:A:581:GLU:HB2	2:B:21:ARG:CA	2.43	0.41
1:A:543:LEU:HD22	1:A:543:LEU:N	2.36	0.41
1:A:751:ASN:HD21	1:A:754:GLN:HB2	1.86	0.41
1:A:734:LYS:HD3	1:A:737:GLU:OE1	2.21	0.41
3:C:699:LEU:HD13	3:C:700:THR:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:6:DA:C2	6:F:7:DA:N6	2.88	0.41
1:A:74:GLN:HB3	1:A:113:HIS:CE1	2.55	0.41
3:C:389:ILE:HD13	3:C:713:ARG:CG	2.45	0.41
1:A:578:LEU:HD13	1:A:591:VAL:HG23	1.99	0.41
1:A:650:ASP:OD1	1:A:650:ASP:N	2.53	0.41
1:A:51:ARG:N	1:A:52:PRO:HD2	2.33	0.41
3:C:457:THR:CG2	3:C:459:PHE:O	2.69	0.41
3:C:413:LEU:HB3	3:C:414:ARG:H	1.69	0.41
3:C:502:SER:O	3:C:503:CYS:CB	2.68	0.41
1:A:578:LEU:HA	2:B:23:GLU:O	2.20	0.41
1:A:587:LYS:HB2	1:A:660:PHE:CZ	2.55	0.41
1:A:428:GLU:HG3	1:A:428:GLU:H	1.63	0.41
1:A:734:LYS:HA	1:A:737:GLU:OE2	2.20	0.41
1:A:735:ARG:HA	1:A:735:ARG:HE	1.84	0.41
1:A:454:LYS:HE2	1:A:490:LYS:HD2	2.02	0.41
1:A:414:ASP:O	1:A:418:ARG:HG3	2.21	0.41
1:A:131:PHE:HZ	1:A:188:VAL:CG2	2.31	0.41
1:A:141:ASP:O	1:A:142:HIS:C	2.58	0.41
3:C:553:SER:HA	3:C:554:PRO:HD3	1.80	0.41
3:C:394:ILE:HD13	3:C:708:GLN:HE22	1.85	0.41
1:A:602:PHE:N	1:A:602:PHE:HD1	2.19	0.41
3:C:498:ILE:N	3:C:498:ILE:CD1	2.84	0.41
3:C:870:VAL:HA	3:C:883:SER:O	2.21	0.41
1:A:558:TYR:O	1:A:562:HIS:HB2	2.21	0.41
1:A:187:MET:O	1:A:191:LYS:HB2	2.22	0.40
1:A:98:VAL:O	1:A:99:SER:C	2.59	0.40
1:A:200:ILE:C	1:A:202:ARG:N	2.74	0.40
3:C:451:PHE:HD1	3:C:470:GLN:CB	2.34	0.40
1:A:533:TRP:HB3	1:A:534:PRO:HD2	2.03	0.40
1:A:748:ASP:HB3	1:A:756:HIS:CE1	2.56	0.40
3:C:184:ASP:CB	3:C:185:PRO:HD2	2.43	0.40
1:A:409:ILE:HG13	1:A:443:ILE:HD11	1.99	0.40
3:C:108:VAL:HG11	3:C:143:ILE:HD11	2.03	0.40
3:C:402:ILE:HG22	3:C:403:ASP:N	2.37	0.40
3:C:184:ASP:N	3:C:187:GLY:O	2.55	0.40
1:A:625:ARG:HD3	1:A:625:ARG:HA	1.91	0.40
1:A:457:LEU:CD2	1:A:461:LEU:HG	2.52	0.40
1:A:390:MET:CE	1:A:391:LYS:HA	2.51	0.40
3:C:643:SER:O	3:C:644:LEU:C	2.59	0.40
3:C:705:ASP:OD1	3:C:705:ASP:C	2.60	0.40
1:A:384:GLU:HA	1:A:387:VAL:HG23	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:561:TRP:O	3:C:587:ILE:HG21	2.19	0.40
1:A:329:VAL:O	1:A:330:ARG:O	2.39	0.40
4:D:218:THR:CG2	4:D:226:VAL:HG13	2.52	0.40
1:A:141:ASP:O	1:A:143:CYS:N	2.55	0.40
1:A:274:VAL:HG21	1:A:283:GLN:HB2	2.04	0.40
3:C:412:PRO:HG2	3:C:412:PRO:O	2.21	0.40
1:A:675:LYS:HD3	1:A:675:LYS:HA	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:ARG:NH1	3:C:769:LYS:NZ[1_565]	2.04	0.16

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	717/742 (97%)	512 (71%)	132 (18%)	73 (10%)	1	13
2	B	19/117 (16%)	14 (74%)	4 (21%)	1 (5%)	2	29
3	C	1095/1159 (94%)	963 (88%)	97 (9%)	35 (3%)	5	41
4	D	353/382 (92%)	326 (92%)	22 (6%)	5 (1%)	14	58
All	All	2184/2400 (91%)	1815 (83%)	255 (12%)	114 (5%)	2	29

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	58	TYR
1	A	76	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	83	LEU
1	A	84	GLU
1	A	127	ASP
1	A	185	ASP
1	A	191	LYS
1	A	207	GLU
1	A	208	ALA
1	A	209	VAL
1	A	276	THR
1	A	330	ARG
1	A	483	CYS
1	A	517	ASP
1	A	587	LYS
1	A	606	ASP
1	A	616	ALA
1	A	633	CYS
1	A	644	LYS
1	A	660	PHE
1	A	661	LYS
1	A	710	LEU
1	A	752	PRO
3	C	367	LEU
3	C	430	VAL
3	C	583	GLY
3	C	598	SER
3	C	672	ASN
3	C	674	LYS
3	C	704	ILE
3	C	705	ASP
3	C	710	LEU
4	D	126	LEU
1	A	96	HIS
1	A	97	LYS
1	A	204	ARG
1	A	229	ASP
1	A	240	ASN
1	A	280	HIS
1	A	441	ARG
1	A	598	VAL
1	A	607	GLY
1	A	652	ASP
1	A	670	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	691	ASP
1	A	711	GLY
3	C	549	SER
3	C	563	ASP
3	C	584	GLY
3	C	855	ASP
3	C	1110	ALA
4	D	120	ALA
1	A	55	PRO
1	A	71	ARG
1	A	75	SER
1	A	82	ASN
1	A	119	LEU
1	A	223	ASP
1	A	350	ALA
1	A	402	PRO
1	A	451	ALA
1	A	586	LYS
1	A	708	LYS
1	A	727	VAL
1	A	757	TYR
1	A	758	VAL
3	C	185	PRO
3	C	418	ASN
3	C	449	MET
3	C	481	GLN
3	C	547	GLY
3	C	562	THR
3	C	624	SER
3	C	644	LEU
3	C	706	GLU
3	C	1109	VAL
1	A	54	LEU
1	A	91	GLU
1	A	189	GLN
1	A	228	LYS
1	A	293	GLN
1	A	325	LEU
1	A	377	GLU
1	A	514	ASN
1	A	610	PHE
1	A	617	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	726	PRO
2	B	37	ILE
3	C	36	ASN
3	C	372	GLN
3	C	488	SER
3	C	503	CYS
4	D	119	HIS
4	D	190	GLY
1	A	51	ARG
1	A	201	GLU
1	A	233	LEU
1	A	378	VAL
1	A	440	PHE
1	A	597	LEU
3	C	242	GLY
3	C	592	LEU
3	C	460	CYS
4	D	291	ASP
3	C	493	PRO
3	C	551	GLY
1	A	306	GLY
1	A	618	GLY
1	A	619	ILE
3	C	406	GLY
3	C	712	ILE
1	A	519	GLY
1	A	405	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	631/674 (94%)	562 (89%)	69 (11%)	8	35
2	B	18/99 (18%)	11 (61%)	7 (39%)	0	0
3	C	957/1015 (94%)	865 (90%)	92 (10%)	10	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	304/335 (91%)	278 (91%)	26 (9%)	13	47
All	All	1910/2123 (90%)	1716 (90%)	194 (10%)	9	37

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	79	ILE
1	A	90	VAL
1	A	93	LEU
1	A	95	SER
1	A	102	LEU
1	A	112	ASP
1	A	124	ASP
1	A	125	SER
1	A	135	ILE
1	A	164	ASN
1	A	171	TRP
1	A	173	MET
1	A	175	LEU
1	A	182	ILE
1	A	183	ILE
1	A	199	LEU
1	A	205	SER
1	A	207	GLU
1	A	217	LEU
1	A	249	ARG
1	A	281	SER
1	A	283	GLN
1	A	292	LYS
1	A	307	LEU
1	A	330	ARG
1	A	353	ILE
1	A	389	LEU
1	A	390	MET
1	A	394	PHE
1	A	402	PRO
1	A	422	LYS
1	A	428	GLU
1	A	429	LEU
1	A	439	LEU
1	A	444	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	450	GLU
1	A	457	LEU
1	A	478	LYS
1	A	483	CYS
1	A	494	MET
1	A	498	MET
1	A	526	ASN
1	A	540	GLU
1	A	546	GLU
1	A	562	HIS
1	A	569	TRP
1	A	591	VAL
1	A	611	GLU
1	A	624	LEU
1	A	626	ARG
1	A	639	LEU
1	A	650	ASP
1	A	652	ASP
1	A	660	PHE
1	A	663	LYS
1	A	665	PHE
1	A	677	THR
1	A	681	GLN
1	A	683	SER
1	A	687	ARG
1	A	691	ASP
1	A	692	ARG
1	A	706	MET
1	A	720	TYR
1	A	726	PRO
1	A	735	ARG
1	A	748	ASP
1	A	751	ASN
2	B	19	LYS
2	B	22	PHE
2	B	25	LYS
2	B	28	ASN
2	B	32	LEU
2	B	37	ILE
2	B	39	VAL
3	C	7	VAL
3	C	81	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	99	ASP
3	C	133	LEU
3	C	159	LEU
3	C	167	VAL
3	C	189	HIS
3	C	191	LYS
3	C	241	ASN
3	C	304	LEU
3	C	314	LEU
3	C	334	VAL
3	C	339	ASP
3	C	360	VAL
3	C	370	GLN
3	C	396	ILE
3	C	403	ASP
3	C	410	LEU
3	C	412	PRO
3	C	414	ARG
3	C	419	ARG
3	C	420	GLU
3	C	452	VAL
3	C	454	ASP
3	C	469	ILE
3	C	473	SER
3	C	476	VAL
3	C	481	GLN
3	C	482	GLU
3	C	487	VAL
3	C	493	PRO
3	C	510	VAL
3	C	518	TYR
3	C	523	PRO
3	C	525	GLU
3	C	531	HIS
3	C	540	CYS
3	C	555	LEU
3	C	560	LEU
3	C	561	TRP
3	C	563	ASP
3	C	567	ARG
3	C	576	LEU
3	C	582	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	587	ILE
3	C	594	THR
3	C	596	PHE
3	C	597	GLU
3	C	602	LEU
3	C	603	LEU
3	C	608	ASP
3	C	614	PHE
3	C	616	LEU
3	C	617	ASN
3	C	618	ILE
3	C	623	LEU
3	C	625	ASP
3	C	627	LYS
3	C	646	THR
3	C	663	ASN
3	C	673	LEU
3	C	688	PRO
3	C	689	ASP
3	C	700	THR
3	C	701	ILE
3	C	703	THR
3	C	704	ILE
3	C	706	GLU
3	C	708	GLN
3	C	713	ARG
3	C	728	GLU
3	C	809	GLN
3	C	820	LYS
3	C	844	LYS
3	C	864	LYS
3	C	867	LYS
3	C	881	LEU
3	C	898	GLU
3	C	899	LEU
3	C	901	THR
3	C	914	LEU
3	C	931	LEU
3	C	957	VAL
3	C	966	LEU
3	C	970	ASN
3	C	984	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	1000	LEU
3	C	1052	LEU
3	C	1086	THR
3	C	1093	LEU
3	C	1106	GLN
3	C	1129	LEU
4	D	111	LYS
4	D	116	GLN
4	D	117	SER
4	D	119	HIS
4	D	126	LEU
4	D	134	LEU
4	D	148	ARG
4	D	174	LEU
4	D	179	VAL
4	D	219	LEU
4	D	243	VAL
4	D	254	THR
4	D	262	LEU
4	D	274	GLU
4	D	293	LEU
4	D	299	VAL
4	D	308	LEU
4	D	312	LYS
4	D	321	MET
4	D	374	LEU
4	D	389	VAL
4	D	393	TYR
4	D	400	LEU
4	D	435	SER
4	D	437	THR
4	D	453	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	92	ASN
1	A	145	GLN
1	A	189	GLN
1	A	283	GLN
1	A	309	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	321	GLN
1	A	333	GLN
1	A	339	HIS
1	A	399	ASN
1	A	412	HIS
1	A	526	ASN
1	A	551	GLN
1	A	570	GLN
1	A	595	GLN
1	A	657	ASN
1	A	673	GLN
1	A	681	GLN
1	A	712	HIS
1	A	722	GLN
1	A	751	ASN
1	A	754	GLN
1	A	756	HIS
2	B	28	ASN
3	C	4	ASN
3	C	30	ASN
3	C	85	ASN
3	C	156	ASN
3	C	186	GLN
3	C	241	ASN
3	C	261	HIS
3	C	374	GLN
3	C	432	GLN
3	C	455	GLN
3	C	462	ASN
3	C	467	GLN
3	C	481	GLN
3	C	494	GLN
3	C	507	GLN
3	C	524	GLN
3	C	536	HIS
3	C	578	HIS
3	C	634	GLN
3	C	648	ASN
3	C	663	ASN
3	C	708	GLN
3	C	727	GLN
3	C	796	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	885	ASN
3	C	904	ASN
3	C	907	ASN
3	C	908	ASN
3	C	1034	ASN
3	C	1055	GLN
4	D	269	HIS
4	D	370	GLN
4	D	453	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	3DR	E	7	5	7,11,12	0.37	0	8,14,17	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3DR	E	7	5	-	0/3/15/16	0/1/1/1

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.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	719/742 (96%)	0.42	44 (6%) 25 25	288, 322, 371, 414	0
2	B	21/117 (17%)	1.13	3 (14%) 4 9	312, 322, 356, 365	0
3	C	1105/1159 (95%)	0.39	47 (4%) 39 37	185, 326, 367, 403	0
4	D	355/382 (92%)	0.32	10 (2%) 56 52	275, 310, 352, 367	0
5	E	11/12 (91%)	1.95	4 (36%) 0 4	342, 359, 437, 441	0
6	F	12/12 (100%)	0.82	1 (8%) 14 17	363, 379, 420, 442	0
All	All	2223/2424 (91%)	0.41	109 (4%) 33 33	185, 322, 367, 442	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	1	DG	6.0
4	D	377	ILE	5.3
1	A	709	THR	4.9
5	E	12	DA	4.7
1	A	183	ILE	4.6
3	C	1015	GLN	4.6
1	A	745	MET	4.4
6	F	12	DC	3.9
1	A	736	ILE	3.7
2	B	27	TRP	3.7
1	A	740	ILE	3.6
3	C	497	ASN	3.6
1	A	182	ILE	3.6
3	C	2	SER	3.5
3	C	1043	LEU	3.4
1	A	97	LYS	3.4
3	C	856	GLY	3.4
3	C	879	LYS	3.4
2	B	19	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	246	LEU	3.3
1	A	128	SER	3.3
3	C	943	GLU	3.3
1	A	420	GLY	3.3
1	A	727	VAL	3.2
1	A	567	LEU	3.2
3	C	766	SER	3.1
3	C	547	GLY	3.1
3	C	771	PHE	3.1
1	A	700	ILE	3.1
4	D	379	ALA	3.0
1	A	710	LEU	3.0
3	C	853	TYR	3.0
3	C	975	PHE	3.0
1	A	294	LEU	2.9
3	C	337	ASN	2.9
1	A	723	LEU	2.8
1	A	578	LEU	2.7
1	A	254	ARG	2.7
1	A	751	ASN	2.6
1	A	704	MET	2.6
3	C	966	LEU	2.6
5	E	2	DC	2.6
3	C	44	VAL	2.6
1	A	523	LEU	2.6
1	A	707	ARG	2.6
3	C	441	GLU	2.6
1	A	224	LEU	2.6
1	A	756	HIS	2.6
1	A	55	PRO	2.6
3	C	16	ASN	2.5
3	C	965	PHE	2.5
4	D	378	LYS	2.5
3	C	942	PHE	2.5
4	D	101	GLY	2.5
3	C	300	LEU	2.4
3	C	855	ASP	2.4
4	D	421	ARG	2.4
1	A	654	PHE	2.4
1	A	754	GLN	2.4
1	A	54	LEU	2.4
3	C	685	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	994	GLU	2.3
1	A	278	LEU	2.3
3	C	979	LYS	2.3
4	D	349	ILE	2.3
4	D	364	ILE	2.3
1	A	661	LYS	2.3
3	C	113	GLY	2.3
1	A	703	ILE	2.3
3	C	17	GLY	2.3
3	C	963	ASP	2.3
3	C	964	ASN	2.3
3	C	43	VAL	2.3
3	C	930	VAL	2.3
3	C	880	LEU	2.2
4	D	363	ILE	2.2
3	C	70	LYS	2.2
3	C	976	VAL	2.2
3	C	546	LEU	2.2
1	A	302	ILE	2.2
3	C	967	GLY	2.2
2	B	24	VAL	2.2
3	C	116	SER	2.2
1	A	581	GLU	2.1
1	A	639	LEU	2.1
1	A	96	HIS	2.1
1	A	697	ASP	2.1
1	A	565	ARG	2.1
3	C	1087	GLY	2.1
3	C	66	LEU	2.1
3	C	977	CYS	2.1
1	A	253	GLU	2.1
3	C	420	GLU	2.1
3	C	442	GLU	2.1
1	A	525	VAL	2.1
3	C	892	GLU	2.1
4	D	393	TYR	2.1
1	A	719	LEU	2.0
3	C	902	GLU	2.0
3	C	237	ILE	2.0
1	A	295	LEU	2.0
3	C	768	SER	2.0
1	A	421	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	230	PHE	2.0
3	C	935	TYR	2.0
1	A	584	GLU	2.0
5	E	8	DA	2.0
1	A	250	LEU	2.0
1	A	419	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
5	3DR	E	7	11/12	0.82	0.25	-	357,362,366,367	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.