



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:59 PM UTC

PDB ID : 3ALX / pdb_00003alx
Title : Crystal structure of the measles virus hemagglutinin bound to its cellular receptor SLAM (MV-H(L482R)-SLAM(N102H/R108Y) fusion)
Authors : Hashiguchi, T.; Ose, T.; Kubota, M.; Maita, N.; Kamishikiryo, J.; Maenaka, K.; Yanagi, Y.
Deposited on : 2010-08-09
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

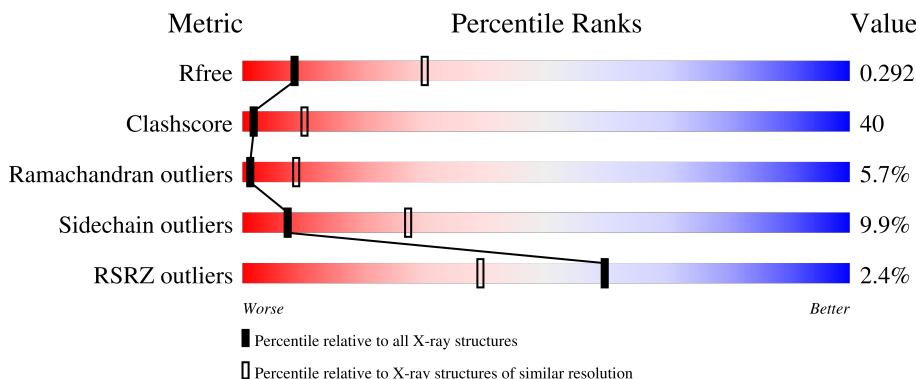
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	
1	B	559	
1	C	559	
1	D	559	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16313 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 Hemagglutinin, LINKER, CDw150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4053	2598	677	750	28			
1	B	526	Total	C	N	O	S	0	0	0
			4141	2651	695	767	28			
1	C	514	Total	C	N	O	S	0	0	0
			4051	2599	676	748	28			
1	D	504	Total	C	N	O	S	0	0	0
			3984	2562	663	732	27			

There are 60 discrepancies between the modelled and reference sequences:

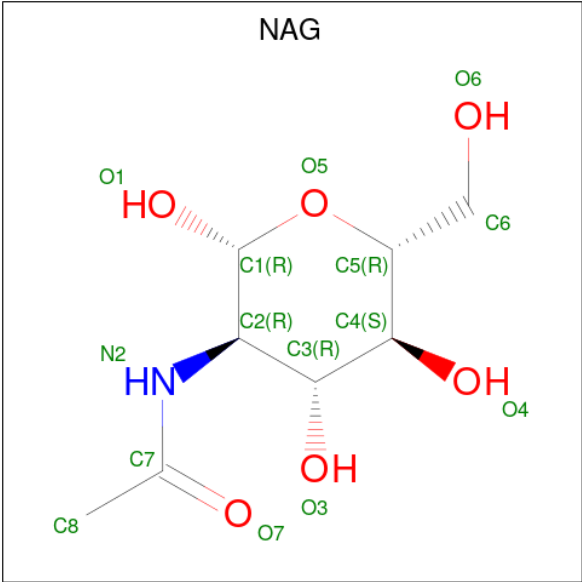
Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	-	expression tag	UNP E2RZS2
A	182	THR	-	expression tag	UNP E2RZS2
A	183	GLY	-	expression tag	UNP E2RZS2
A	482	ARG	LEU	engineered mutation	UNP E2RZS2
A	102	HIS	ASN	engineered mutation	UNP Q9GJT3
A	108	TYR	ARG	engineered mutation	UNP Q9GJT3
A	141	GLY	-	expression tag	UNP Q9GJT3
A	142	THR	-	expression tag	UNP Q9GJT3
A	143	LYS	-	expression tag	UNP Q9GJT3
A	144	HIS	-	expression tag	UNP Q9GJT3
A	145	HIS	-	expression tag	UNP Q9GJT3
A	146	HIS	-	expression tag	UNP Q9GJT3
A	147	HIS	-	expression tag	UNP Q9GJT3
A	148	HIS	-	expression tag	UNP Q9GJT3
A	149	HIS	-	expression tag	UNP Q9GJT3
B	181	GLU	-	expression tag	UNP E2RZS2
B	182	THR	-	expression tag	UNP E2RZS2
B	183	GLY	-	expression tag	UNP E2RZS2
B	482	ARG	LEU	engineered mutation	UNP E2RZS2
B	102	HIS	ASN	engineered mutation	UNP Q9GJT3
B	108	TYR	ARG	engineered mutation	UNP Q9GJT3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	141	GLY	-	expression tag	UNP Q9GJT3
B	142	THR	-	expression tag	UNP Q9GJT3
B	143	LYS	-	expression tag	UNP Q9GJT3
B	144	HIS	-	expression tag	UNP Q9GJT3
B	145	HIS	-	expression tag	UNP Q9GJT3
B	146	HIS	-	expression tag	UNP Q9GJT3
B	147	HIS	-	expression tag	UNP Q9GJT3
B	148	HIS	-	expression tag	UNP Q9GJT3
B	149	HIS	-	expression tag	UNP Q9GJT3
C	181	GLU	-	expression tag	UNP E2RZS2
C	182	THR	-	expression tag	UNP E2RZS2
C	183	GLY	-	expression tag	UNP E2RZS2
C	482	ARG	LEU	engineered mutation	UNP E2RZS2
C	102	HIS	ASN	engineered mutation	UNP Q9GJT3
C	108	TYR	ARG	engineered mutation	UNP Q9GJT3
C	141	GLY	-	expression tag	UNP Q9GJT3
C	142	THR	-	expression tag	UNP Q9GJT3
C	143	LYS	-	expression tag	UNP Q9GJT3
C	144	HIS	-	expression tag	UNP Q9GJT3
C	145	HIS	-	expression tag	UNP Q9GJT3
C	146	HIS	-	expression tag	UNP Q9GJT3
C	147	HIS	-	expression tag	UNP Q9GJT3
C	148	HIS	-	expression tag	UNP Q9GJT3
C	149	HIS	-	expression tag	UNP Q9GJT3
D	181	GLU	-	expression tag	UNP E2RZS2
D	182	THR	-	expression tag	UNP E2RZS2
D	183	GLY	-	expression tag	UNP E2RZS2
D	482	ARG	LEU	engineered mutation	UNP E2RZS2
D	102	HIS	ASN	engineered mutation	UNP Q9GJT3
D	108	TYR	ARG	engineered mutation	UNP Q9GJT3
D	141	GLY	-	expression tag	UNP Q9GJT3
D	142	THR	-	expression tag	UNP Q9GJT3
D	143	LYS	-	expression tag	UNP Q9GJT3
D	144	HIS	-	expression tag	UNP Q9GJT3
D	145	HIS	-	expression tag	UNP Q9GJT3
D	146	HIS	-	expression tag	UNP Q9GJT3
D	147	HIS	-	expression tag	UNP Q9GJT3
D	148	HIS	-	expression tag	UNP Q9GJT3
D	149	HIS	-	expression tag	UNP Q9GJT3

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

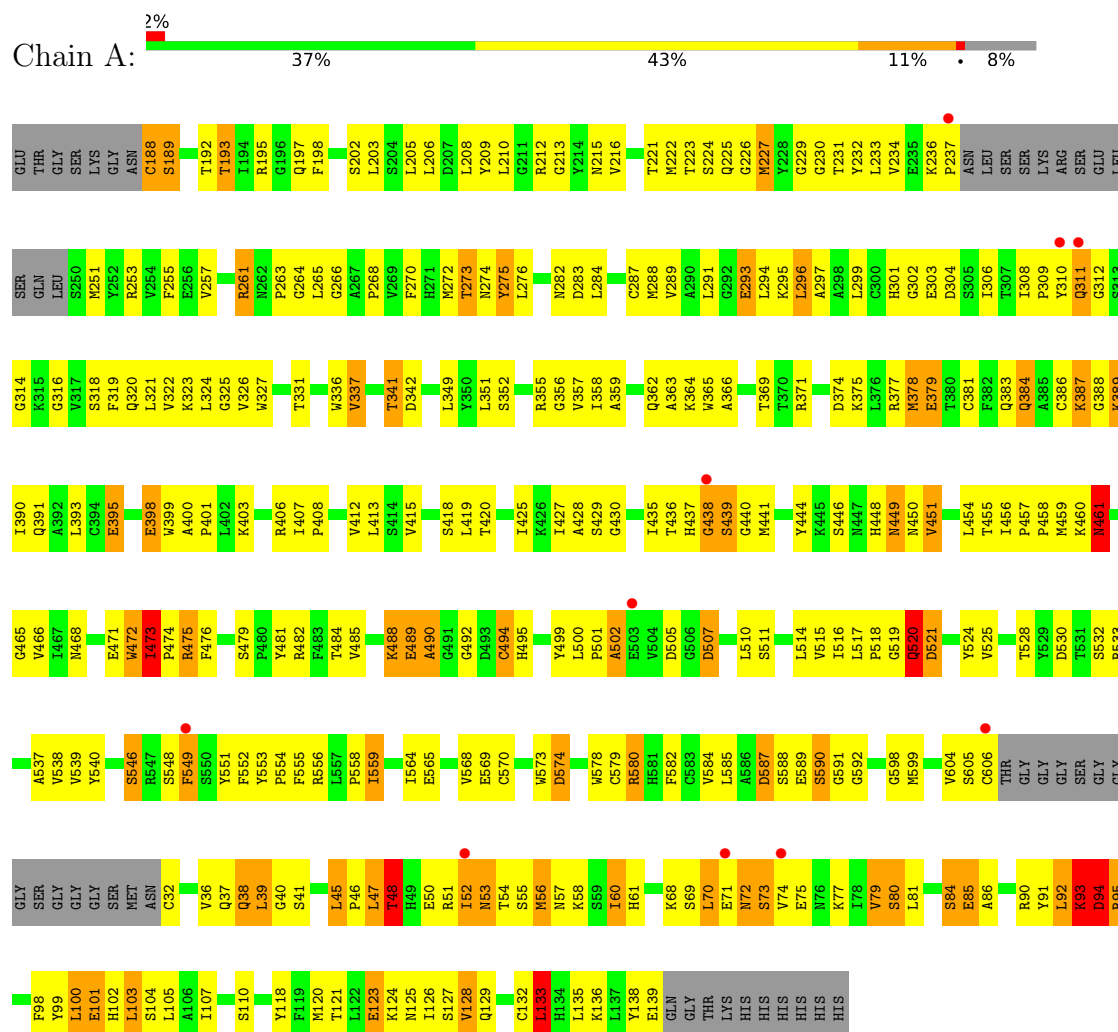


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

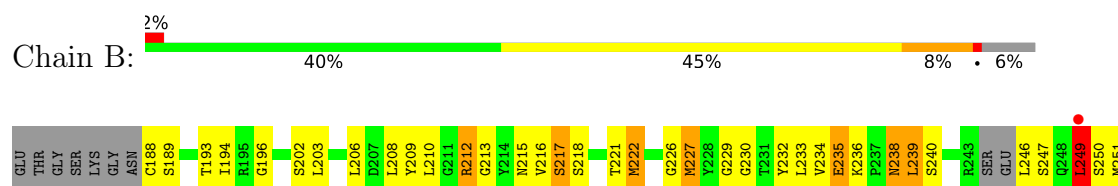
3 Residue-property plots

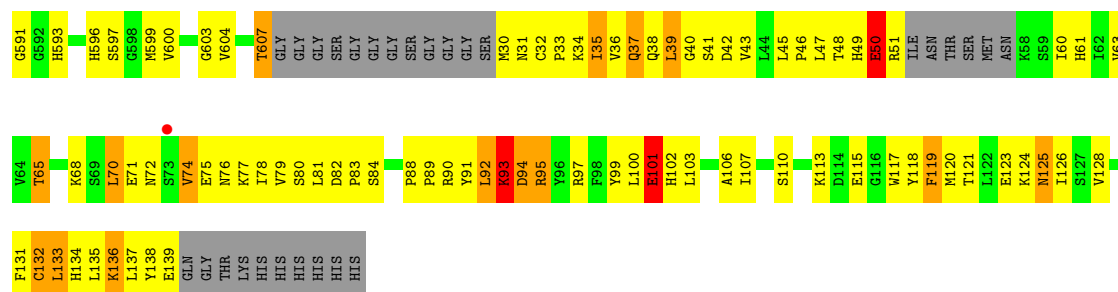
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hemagglutinin, LINKER, CDw150

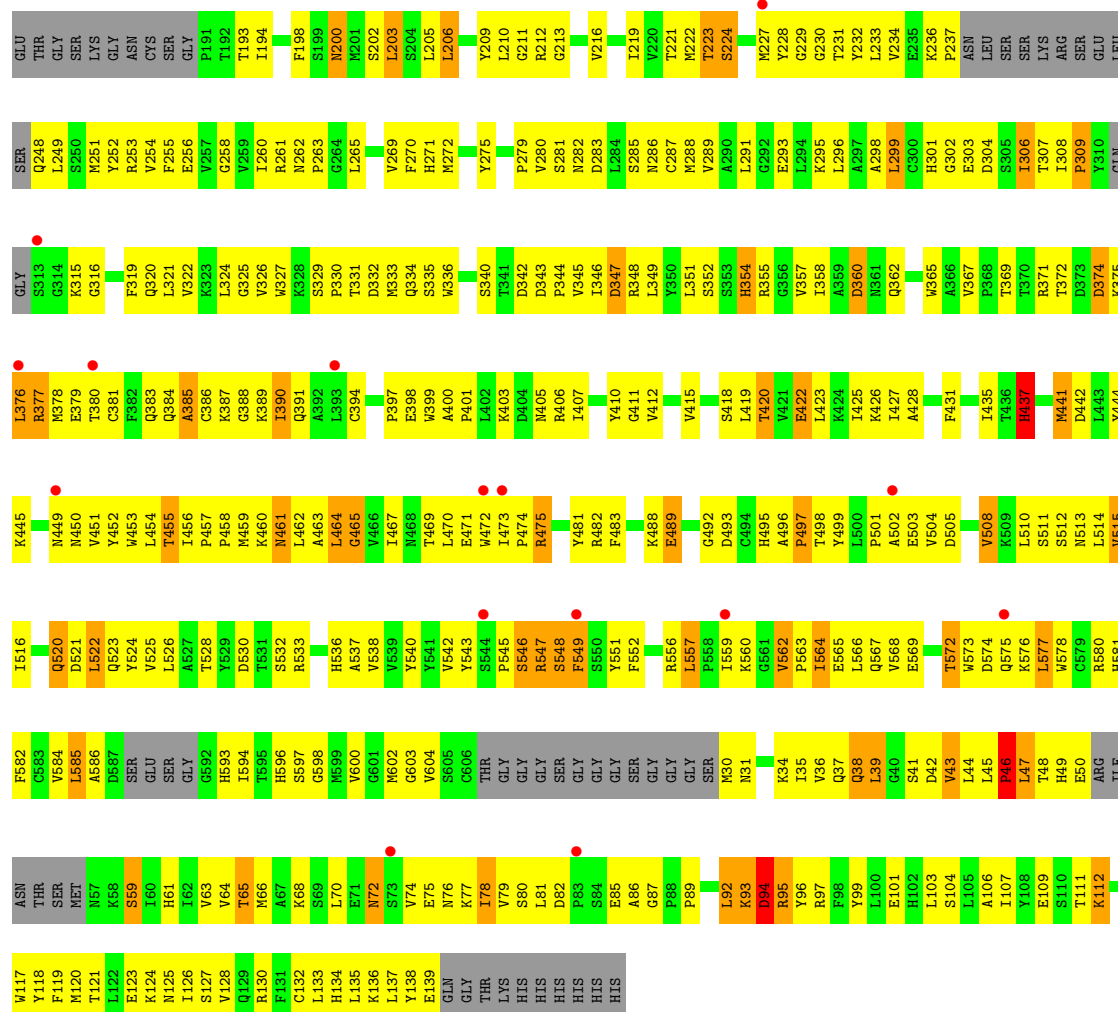


• Molecule 1: Hemagglutinin, LINKER, CDw150





• Molecule 1: Hemagglutinin, LINKER, CDw150



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.71Å 170.07Å 110.68Å 90.00° 117.28° 90.00°	Depositor
Resolution (Å)	19.97 – 3.15 19.97 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.97-3.15) 98.8 (19.97-3.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.15Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.231 , 0.292 0.232 , 0.292	Depositor DCC
R_{free} test set	2644 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16313	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.25% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.61	1/4155 (0.0%)	1.06	20/5646 (0.4%)
1	B	0.54	1/4243 (0.0%)	1.04	20/5763 (0.3%)
1	C	0.56	0/4151	1.04	18/5638 (0.3%)
1	D	0.50	0/4083	0.99	14/5545 (0.3%)
All	All	0.55	2/16632 (0.0%)	1.03	72/22592 (0.3%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	MET	SD-CE	6.96	1.97	1.79
1	B	227	MET	SD-CE	5.24	1.92	1.79

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	LEU	N-CA-C	-13.15	96.54	112.59
1	A	92	LEU	N-CA-C	-12.63	96.58	112.88
1	C	92	LEU	N-CA-C	-9.62	101.47	113.02
1	B	48	THR	N-CA-C	-9.30	94.02	109.46
1	A	520	GLN	N-CA-C	-9.29	102.52	112.93
1	A	48	THR	N-CA-C	-8.60	96.09	109.76
1	D	78	ILE	N-CA-C	-8.51	104.45	112.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	ILE	N-CA-C	-8.41	105.09	111.90
1	C	536	HIS	N-CA-C	-7.93	100.65	110.41
1	C	189	SER	N-CA-C	-7.48	104.12	113.18
1	B	240	SER	N-CA-C	-7.21	105.02	113.88
1	A	337	VAL	CA-C-N	7.11	127.67	120.14
1	A	337	VAL	C-N-CA	7.11	127.67	120.14
1	B	439	SER	N-CA-C	-6.86	104.92	113.28
1	A	420	THR	N-CA-C	-6.79	104.81	113.23
1	B	347	ASP	N-CA-C	6.71	118.48	111.03
1	A	123	GLU	N-CA-C	6.66	119.80	109.07
1	A	54	THR	N-CA-C	-6.62	103.61	112.94
1	D	562	VAL	N-CA-C	6.59	114.65	107.60
1	D	420	THR	N-CA-C	-6.44	103.77	111.69
1	C	236	LYS	N-CA-C	6.38	123.92	109.81
1	B	575	GLN	N-CA-C	6.29	120.25	112.58
1	B	96	TYR	N-CA-C	6.22	119.73	110.52
1	A	342	ASP	N-CA-C	-6.22	105.52	113.23
1	D	203	LEU	N-CA-C	-6.19	103.03	112.99
1	C	325	GLY	N-CA-C	-6.11	104.38	112.82
1	B	249	LEU	N-CA-C	-6.11	105.96	113.41
1	C	547	ARG	CB-CA-C	-6.10	108.94	117.23
1	A	460	LYS	CB-CA-C	-6.06	109.57	116.54
1	D	132	CYS	N-CA-C	6.02	119.01	109.50
1	B	485	VAL	CA-C-N	5.96	125.72	119.76
1	B	485	VAL	C-N-CA	5.96	125.72	119.76
1	A	93	LYS	N-CA-C	5.91	123.39	110.80
1	A	537	ALA	N-CA-C	5.89	117.73	108.96
1	C	119	PHE	N-CA-C	5.89	118.32	108.02
1	A	94	ASP	N-CA-C	-5.85	98.34	110.80
1	B	337	VAL	N-CA-C	5.79	114.63	108.95
1	B	420	THR	N-CA-C	-5.74	106.11	113.23
1	A	461	ASN	N-CA-C	-5.71	105.90	112.92
1	B	460	LYS	CB-CA-C	-5.69	110.00	116.54
1	D	94	ASP	N-CA-C	5.69	122.91	110.80
1	A	304	ASP	N-CA-C	-5.69	106.69	113.97
1	B	456	ILE	CA-C-N	5.66	123.80	119.66
1	B	456	ILE	C-N-CA	5.66	123.80	119.66
1	C	78	ILE	CB-CA-C	-5.66	105.87	111.30
1	B	513	ASN	N-CA-C	-5.65	103.25	110.53
1	A	507	ASP	N-CA-C	-5.59	105.58	112.90
1	A	605	SER	N-CA-C	5.57	116.99	108.42
1	C	335	SER	N-CA-C	5.52	117.79	109.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	562	VAL	CA-C-N	5.52	125.69	119.90
1	D	562	VAL	C-N-CA	5.52	125.69	119.90
1	B	81	LEU	N-CA-C	5.49	116.87	108.42
1	D	385	ALA	N-CA-C	-5.46	106.46	113.23
1	C	343	ASP	CA-C-N	5.44	125.15	119.82
1	C	343	ASP	C-N-CA	5.44	125.15	119.82
1	A	546	SER	N-CA-C	-5.40	104.43	111.02
1	B	72	ASN	N-CA-C	-5.37	104.00	111.52
1	A	465	GLY	N-CA-C	-5.36	104.11	112.58
1	D	354	HIS	N-CA-C	5.35	117.14	108.26
1	B	51	ARG	N-CA-C	-5.30	105.08	112.45
1	D	585	LEU	N-CA-C	5.30	118.01	108.48
1	C	262	ASN	CA-C-N	5.29	126.45	119.84
1	C	262	ASN	C-N-CA	5.29	126.45	119.84
1	C	337	VAL	CA-C-N	5.22	125.67	120.14
1	C	337	VAL	C-N-CA	5.22	125.67	120.14
1	B	212	ARG	N-CA-C	-5.22	106.60	113.17
1	D	508	VAL	N-CA-C	-5.22	99.59	107.73
1	A	587	ASP	N-CA-C	5.18	116.78	110.41
1	C	42	ASP	N-CA-C	-5.14	103.53	110.68
1	D	536	HIS	N-CA-C	-5.13	103.37	110.35
1	C	475	ARG	N-CA-C	-5.11	99.92	110.80
1	D	564	ILE	N-CA-C	-5.03	107.80	112.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	541	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4053	0	4023	306	0
1	B	4141	0	4119	320	0
1	C	4051	0	4024	335	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3984	0	3964	359	0
2	A	14	0	13	0	0
2	B	28	0	26	0	0
2	C	28	0	26	1	0
2	D	14	0	13	1	0
All	All	16313	0	16208	1295	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 40.

All (1295) 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:85:GLU:HG2	1:A:86:ALA:H	1.09	1.16
1:A:236:LYS:HB3	1:A:237:PRO:HD2	1.30	1.14
1:D:503:GLU:HB2	1:D:76:ASN:HD22	1.05	1.09
1:A:60:ILE:HG22	1:A:61:HIS:H	1.13	1.08
1:A:540:TYR:HE1	1:A:568:VAL:HG21	1.22	1.04
1:C:546:SER:HB3	1:C:547:ARG:HH21	1.15	1.04
1:C:251:MET:HE3	1:C:283:ASP:HB3	1.40	1.00
1:C:194:ILE:HG13	1:C:604:VAL:HG12	1.44	0.98
1:D:37:GLN:HE22	1:D:43:VAL:HA	1.28	0.97
1:D:457:PRO:HB3	1:D:513:ASN:HA	1.49	0.95
1:D:503:GLU:HB2	1:D:76:ASN:ND2	1.82	0.94
1:A:589:GLU:HG3	1:A:590:SER:H	1.34	0.93
1:D:37:GLN:NE2	1:D:43:VAL:HA	1.84	0.92
1:C:546:SER:HB3	1:C:547:ARG:NH2	1.84	0.91
1:B:74:VAL:HG13	1:B:75:GLU:H	1.33	0.90
1:B:558:PRO:HG2	1:B:559:ILE:HG23	1.52	0.90
1:D:194:ILE:HG13	1:D:604:VAL:HG12	1.55	0.89
1:C:306:ILE:HD13	1:C:351:LEU:HD21	1.55	0.89
1:C:237:PRO:HG2	1:C:249:LEU:HA	1.54	0.89
1:B:472:TRP:HE3	1:B:472:TRP:H	1.19	0.88
1:B:473:ILE:HB	1:B:474:PRO:HD3	1.55	0.88
1:D:222:MET:HE2	1:D:291:LEU:HB2	1.53	0.87
1:D:47:LEU:HD13	1:D:120:MET:HB2	1.56	0.87
1:B:472:TRP:HA	1:B:476:PHE:HA	1.57	0.86
1:C:81:LEU:HD23	1:C:89:PRO:HB3	1.56	0.85
1:D:520:GLN:H	1:D:520:GLN:NE2	1.73	0.85
1:B:93:LYS:HD2	1:B:94:ASP:C	2.01	0.85
1:D:458:PRO:HG2	1:D:511:SER:HB3	1.58	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:HIS:HB3	1:D:459:MET:HG2	1.58	0.85
1:B:430:GLY:HA3	1:B:476:PHE:HE2	1.42	0.84
1:B:475:ARG:NH1	1:B:477:LYS:HD3	1.91	0.84
1:C:457:PRO:HB3	1:C:513:ASN:HA	1.58	0.84
1:A:85:GLU:HG2	1:A:86:ALA:N	1.92	0.84
1:A:540:TYR:CE1	1:A:568:VAL:HG21	2.12	0.83
1:B:562:VAL:HB	1:B:586:ALA:HB3	1.60	0.83
1:D:93:LYS:HA	1:D:93:LYS:NZ	1.93	0.83
1:D:121:THR:HG23	1:D:128:VAL:HG13	1.59	0.82
1:B:400:ALA:HB3	1:B:401:PRO:HD3	1.60	0.82
1:B:216:VAL:HG22	1:B:234:VAL:HG12	1.61	0.82
1:A:236:LYS:HB3	1:A:237:PRO:CD	2.10	0.82
1:C:135:LEU:HD23	1:C:136:LYS:N	1.95	0.82
1:B:464:LEU:HG	1:B:465:GLY:H	1.45	0.81
1:D:286:ASN:ND2	1:D:304:ASP:HB3	1.95	0.81
1:A:60:ILE:HG22	1:A:61:HIS:N	1.95	0.81
1:C:36:VAL:HG12	1:C:136:LYS:HB3	1.63	0.81
1:A:450:ASN:HA	1:A:472:TRP:CH2	2.16	0.80
1:B:89:PRO:HG2	1:B:91:TYR:CE2	2.17	0.80
1:D:261:ARG:NH1	1:D:261:ARG:HB2	1.97	0.80
1:C:390:ILE:HG23	1:C:393:LEU:HB2	1.64	0.80
1:C:531:THR:HG22	1:C:536:HIS:CD2	2.17	0.79
1:C:47:LEU:HD13	1:C:120:MET:HB2	1.65	0.79
1:C:378:MET:HB2	1:C:407:ILE:HG21	1.64	0.78
1:D:123:GLU:HB3	1:D:128:VAL:HG22	1.63	0.78
1:C:252:TYR:CE1	1:C:279:PRO:HG3	2.17	0.78
1:A:93:LYS:HD2	1:A:94:ASP:H	1.48	0.78
1:C:296:LEU:HD23	1:C:296:LEU:O	1.83	0.78
1:D:537:ALA:HA	1:D:557:LEU:HD22	1.64	0.78
1:C:545:PRO:HB3	1:C:71:GLU:HA	1.64	0.78
1:D:503:GLU:CB	1:D:76:ASN:HD22	1.91	0.77
1:A:93:LYS:HD2	1:A:94:ASP:C	2.09	0.77
1:C:33:PRO:HD2	1:C:132:CYS:SG	2.25	0.77
1:C:93:LYS:HD2	1:C:94:ASP:N	2.00	0.77
1:A:378:MET:HB3	1:A:407:ILE:HG21	1.68	0.77
1:D:38:GLN:HB3	1:D:41:SER:OG	1.85	0.76
1:B:236:LYS:HE3	1:B:238:ASN:HB3	1.65	0.76
1:A:374:ASP:HB2	1:A:407:ILE:HB	1.65	0.76
1:C:68:LYS:HD2	1:C:115:GLU:O	1.86	0.76
1:A:36:VAL:HA	1:A:136:LYS:O	1.84	0.76
1:C:205:LEU:HB2	1:C:272:MET:HE1	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:O	1:A:72:ASN:HB2	1.85	0.76
1:A:461:ASN:H	1:A:461:ASN:ND2	1.83	0.76
1:B:77:LYS:HB3	1:B:92:LEU:HD11	1.68	0.76
1:D:525:VAL:HG12	1:D:542:VAL:HA	1.67	0.76
1:A:274:ASN:HD22	1:A:324:LEU:HB3	1.51	0.75
1:A:378:MET:HE3	1:A:378:MET:HA	1.68	0.75
1:D:464:LEU:HG	1:D:465:GLY:H	1.50	0.75
1:D:37:GLN:CD	1:D:43:VAL:HG23	2.10	0.75
1:C:384:GLN:HE22	1:C:490:ALA:HA	1.51	0.75
1:D:35:ILE:HD11	1:D:45:LEU:HG	1.68	0.75
1:C:194:ILE:CG1	1:C:604:VAL:HG12	2.17	0.75
1:A:461:ASN:H	1:A:461:ASN:HD22	1.34	0.75
1:A:84:SER:O	1:A:85:GLU:HB2	1.85	0.75
1:B:95:ARG:HG3	1:B:95:ARG:HH11	1.51	0.74
1:D:309:PRO:HG3	1:D:316:GLY:HA2	1.69	0.74
1:A:473:ILE:HG22	1:A:474:PRO:N	2.02	0.74
1:D:343:ASP:OD1	1:D:345:VAL:HG12	1.86	0.74
1:D:237:PRO:HA	1:D:249:LEU:HD23	1.69	0.74
1:D:540:TYR:HE1	1:D:568:VAL:HG21	1.53	0.74
1:A:231:THR:HG21	1:A:287:CYS:HB2	1.69	0.74
1:B:139:GLU:O	1:B:140:GLN:HB2	1.87	0.73
1:D:205:LEU:HB2	1:D:272:MET:HE1	1.68	0.73
1:A:556:ARG:HH12	1:A:125:ASN:HA	1.53	0.73
1:B:140:GLN:HG3	1:C:421:VAL:HA	1.68	0.73
1:A:93:LYS:HD2	1:A:94:ASP:N	2.03	0.73
1:B:570:CYS:HB3	1:B:577:LEU:HD21	1.71	0.73
1:D:354:HIS:CE1	1:D:367:VAL:HG12	2.24	0.73
1:A:580:ARG:HB3	1:A:599:MET:HE3	1.70	0.73
1:A:580:ARG:HH11	1:A:580:ARG:HG3	1.53	0.73
1:A:40:GLY:HA2	1:A:110:SER:O	1.88	0.73
1:B:93:LYS:HD2	1:B:94:ASP:H	1.53	0.73
1:C:378:MET:CB	1:C:407:ILE:HG21	2.19	0.73
1:A:222:MET:HB3	1:A:355:ARG:HD3	1.71	0.72
1:B:481:TYR:O	1:B:482:ARG:HG2	1.90	0.72
1:D:72:ASN:N	1:D:72:ASN:HD22	1.86	0.72
1:A:326:VAL:HG23	1:A:327:TRP:CD1	2.25	0.72
1:B:464:LEU:HG	1:B:465:GLY:N	2.04	0.72
1:D:93:LYS:HG3	1:D:94:ASP:H	1.54	0.72
1:A:459:MET:HA	1:A:459:MET:HE2	1.69	0.72
1:B:35:ILE:HG13	1:B:35:ILE:O	1.89	0.72
1:B:91:TYR:HB3	1:B:93:LYS:HB3	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:GLU:HG3	1:D:304:ASP:H	1.54	0.72
1:B:103:LEU:HD13	1:B:120:MET:HE1	1.70	0.72
1:C:77:LYS:HD2	1:C:80:SER:OG	1.89	0.72
1:A:60:ILE:CG2	1:A:61:HIS:H	1.97	0.72
1:D:65:THR:HG23	1:D:119:PHE:HB2	1.71	0.72
1:B:227:MET:HE1	1:B:294:LEU:H	1.55	0.72
1:C:216:VAL:HG22	1:C:234:VAL:HG13	1.71	0.72
1:C:45:LEU:HD21	1:C:135:LEU:HD12	1.70	0.72
1:B:340:SER:HB3	1:B:426:LYS:HA	1.72	0.72
1:B:461:ASN:H	1:B:461:ASN:HD22	1.35	0.72
1:B:378:MET:CB	1:B:407:ILE:HG21	2.19	0.71
1:A:552:PHE:HE1	1:A:121:THR:HG1	1.37	0.71
1:C:528:THR:HG22	1:C:539:VAL:HB	1.71	0.71
1:C:308:ILE:HD11	1:C:349:LEU:HD12	1.71	0.71
1:D:219:ILE:HD12	1:D:219:ILE:H	1.56	0.71
1:A:540:TYR:O	1:A:552:PHE:HA	1.91	0.71
1:A:585:LEU:HD23	1:A:585:LEU:H	1.55	0.71
1:B:529:TYR:CD1	1:B:563:PRO:HG3	2.26	0.71
1:A:556:ARG:NH1	1:A:125:ASN:HA	2.06	0.71
1:B:288:MET:HE3	1:B:299:LEU:HB3	1.73	0.71
1:B:337:VAL:HG12	1:B:423:LEU:HB3	1.72	0.71
1:D:378:MET:HB3	1:D:407:ILE:HG21	1.72	0.71
1:A:398:GLU:O	1:A:403:LYS:HE3	1.91	0.70
1:B:74:VAL:HG13	1:B:75:GLU:N	2.03	0.70
1:D:97:ARG:HB3	1:D:106:ALA:HB3	1.71	0.70
1:A:70:LEU:HD22	1:A:70:LEU:H	1.56	0.70
1:B:458:PRO:HG3	1:B:465:GLY:H	1.54	0.70
1:D:253:ARG:HH21	1:D:285:SER:HB2	1.56	0.70
1:C:216:VAL:HG22	1:C:234:VAL:CG1	2.21	0.70
1:D:545:PRO:C	1:D:547:ARG:H	1.99	0.69
1:C:587:ASP:O	1:C:591:GLY:HA2	1.92	0.69
1:B:399:TRP:CD1	1:B:401:PRO:HD2	2.27	0.69
1:D:211:GLY:C	1:D:213:GLY:H	2.01	0.69
1:B:101:GLU:CD	1:B:101:GLU:H	2.00	0.69
1:C:222:MET:HB3	1:C:355:ARG:HD3	1.74	0.69
1:B:346:ILE:HG23	1:B:369:THR:HG21	1.73	0.69
1:D:306:ILE:N	1:D:306:ILE:HD12	2.08	0.69
1:B:544:SER:HB2	1:B:549:PHE:HB3	1.73	0.69
1:D:415:VAL:HG12	1:D:425:ILE:HA	1.75	0.68
1:C:305:SER:C	1:C:306:ILE:HD12	2.19	0.68
1:C:464:LEU:CD2	1:C:498:THR:HB	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ILE:HG12	1:D:551:TYR:CD2	2.28	0.68
1:D:564:ILE:HD12	1:D:564:ILE:O	1.93	0.68
1:A:272:MET:HE3	1:A:275:TYR:HB3	1.76	0.68
1:C:461:ASN:C	1:C:461:ASN:HD22	2.01	0.68
1:C:89:PRO:HG2	1:C:91:TYR:CE2	2.27	0.68
1:D:216:VAL:HG22	1:D:234:VAL:HG22	1.75	0.68
1:A:222:MET:HE2	1:A:291:LEU:HB2	1.76	0.68
1:C:406:ARG:O	1:C:408:PRO:HD3	1.92	0.68
1:C:261:ARG:HH11	1:C:271:HIS:HB3	1.59	0.67
1:B:348:ARG:HD3	1:B:350:TYR:OH	1.94	0.67
1:C:389:LYS:HE3	1:C:500:LEU:H	1.58	0.67
1:C:43:VAL:CG2	1:C:107:ILE:HB	2.24	0.67
1:B:475:ARG:O	1:B:476:PHE:HB3	1.95	0.67
1:B:62:ILE:HD13	1:B:83:PRO:HD3	1.75	0.67
1:D:194:ILE:N	1:D:194:ILE:HD12	2.09	0.67
1:A:236:LYS:CB	1:A:237:PRO:HD2	2.16	0.67
1:A:461:ASN:HD22	1:A:461:ASN:N	1.88	0.67
1:D:458:PRO:HG2	1:D:511:SER:CB	2.25	0.67
1:B:74:VAL:O	1:B:75:GLU:HB3	1.94	0.67
1:D:288:MET:HB3	1:D:365:TRP:NE1	2.10	0.67
1:D:384:GLN:HA	1:D:387:LYS:HE3	1.77	0.66
1:C:37:GLN:HG2	1:C:43:VAL:HG12	1.77	0.66
1:A:224:SER:O	1:A:225:GLN:HB2	1.95	0.66
1:B:549:PHE:HD1	1:B:549:PHE:O	1.78	0.66
1:D:261:ARG:HH11	1:D:261:ARG:CB	2.09	0.66
1:A:52:ILE:HD13	1:D:282:ASN:HD21	1.60	0.66
1:C:326:VAL:HG13	1:C:327:TRP:H	1.61	0.66
1:C:546:SER:CB	1:C:547:ARG:HH21	2.02	0.66
1:C:353:SER:OG	1:C:567:GLN:NE2	2.29	0.66
1:D:512:SER:HA	1:D:566:LEU:O	1.96	0.66
1:B:499:TYR:CD2	1:B:501:PRO:HD3	2.30	0.66
1:D:293:GLU:CD	1:D:360:ASP:H	2.04	0.65
1:D:77:LYS:HD2	1:D:80:SER:OG	1.96	0.65
1:A:448:HIS:HB2	1:A:451:VAL:CG1	2.26	0.65
1:A:91:TYR:HB3	1:A:93:LYS:HB3	1.77	0.65
1:B:430:GLY:CA	1:B:476:PHE:HE2	2.09	0.65
1:B:461:ASN:H	1:B:461:ASN:ND2	1.92	0.65
1:A:585:LEU:HD23	1:A:585:LEU:N	2.12	0.65
1:C:82:ASP:OD2	1:C:84:SER:HB3	1.96	0.65
1:D:514:LEU:CD1	1:D:526:LEU:HD23	2.26	0.65
1:D:521:ASP:HB2	1:D:546:SER:HB2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:HG13	1:D:107:ILE:HB	1.79	0.65
1:B:140:GLN:HE21	1:C:421:VAL:HA	1.62	0.65
1:D:289:VAL:HG13	1:D:296:LEU:HD11	1.78	0.65
1:A:499:TYR:CD2	1:A:501:PRO:HD3	2.32	0.65
1:A:51:ARG:HH12	1:A:102:HIS:HB3	1.62	0.65
1:B:461:ASN:HD22	1:B:461:ASN:N	1.91	0.65
1:C:273:THR:O	1:C:274:ASN:HB2	1.97	0.65
1:A:430:GLY:HA3	1:A:476:PHE:CE2	2.33	0.64
1:B:369:THR:O	1:B:409:SER:HB3	1.97	0.64
1:C:439:SER:HB2	1:C:457:PRO:HG2	1.78	0.64
1:B:216:VAL:HA	1:B:233:LEU:O	1.97	0.64
1:B:467:ILE:O	1:B:481:TYR:HB3	1.96	0.64
1:B:583:CYS:O	1:B:595:THR:HA	1.96	0.64
1:A:52:ILE:CD1	1:D:282:ASN:HD21	2.10	0.64
1:A:520:GLN:HG3	1:A:520:GLN:O	1.97	0.64
1:A:589:GLU:CG	1:A:590:SER:H	2.07	0.64
1:B:215:ASN:CB	1:B:235:GLU:HB2	2.27	0.64
1:B:61:HIS:CE1	1:B:63:VAL:HG22	2.33	0.64
1:B:343:ASP:OD2	1:B:346:ILE:HG13	1.97	0.64
1:B:93:LYS:CG	1:B:94:ASP:N	2.60	0.64
1:B:378:MET:HB2	1:B:407:ILE:HG21	1.79	0.64
1:D:377:ARG:HG3	1:D:377:ARG:HH11	1.63	0.64
1:B:533:ARG:HG2	1:B:61:HIS:CD2	2.32	0.64
1:C:107:ILE:HD11	1:C:118:TYR:CE2	2.32	0.64
1:D:547:ARG:HG3	1:D:548:SER:H	1.63	0.64
1:A:337:VAL:CG1	1:A:425:ILE:HG13	2.28	0.64
1:D:206:LEU:HG	1:D:232:TYR:CE2	2.33	0.64
1:C:410:TYR:CE1	1:C:435:ILE:HD11	2.32	0.63
1:C:65:THR:HG21	1:C:75:GLU:HB3	1.81	0.63
1:C:473:ILE:HG22	1:C:474:PRO:HD3	1.80	0.63
1:A:521:ASP:CG	1:A:546:SER:HB2	2.23	0.63
1:A:56:MET:HG2	1:A:57:ASN:H	1.62	0.63
1:B:557:LEU:HD23	1:B:559:ILE:HD11	1.79	0.63
1:D:533:ARG:HB3	1:D:61:HIS:CD2	2.34	0.63
1:A:580:ARG:HH11	1:A:580:ARG:CG	2.12	0.63
1:D:467:ILE:O	1:D:481:TYR:HB3	1.98	0.63
1:A:309:PRO:HG3	1:A:316:GLY:HA3	1.80	0.63
1:B:188:CYS:O	1:B:189:SER:HB3	1.99	0.63
1:B:352:SER:N	1:B:354:HIS:NE2	2.46	0.63
1:A:358:ILE:HA	1:A:362:GLN:O	1.98	0.63
1:B:386:CYS:HA	1:B:390:ILE:HG13	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:HB2	1:D:252:TYR:OH	1.98	0.63
1:D:38:GLN:HB3	1:D:41:SER:CB	2.29	0.63
1:C:505:ASP:HB3	1:C:508:VAL:HG12	1.80	0.62
1:C:580:ARG:HE	1:C:599:MET:HE3	1.64	0.62
1:A:559:ILE:HD13	1:A:559:ILE:H	1.64	0.62
1:A:448:HIS:HB2	1:A:451:VAL:HG12	1.81	0.62
1:C:526:LEU:HD12	1:C:526:LEU:C	2.24	0.62
1:A:375:LYS:O	1:A:379:GLU:HB2	1.99	0.62
1:A:517:LEU:HD11	1:A:525:VAL:CG2	2.28	0.62
1:B:74:VAL:CG1	1:B:75:GLU:H	2.11	0.62
1:D:449:ASN:O	1:D:450:ASN:HB2	2.00	0.62
1:B:36:VAL:HA	1:B:136:LYS:O	1.99	0.62
1:B:93:LYS:HD2	1:B:95:ARG:N	2.15	0.62
1:D:124:LYS:HE3	1:D:125:ASN:OD1	1.99	0.62
1:B:357:VAL:HG21	1:B:452:TYR:HE1	1.64	0.62
1:D:526:LEU:C	1:D:526:LEU:HD12	2.25	0.62
1:C:293:GLU:CB	1:C:295:LYS:HE2	2.30	0.62
1:A:309:PRO:HB2	1:A:341:THR:HG21	1.82	0.62
1:B:229:GLY:N	1:B:291:LEU:HD11	2.14	0.62
1:D:101:GLU:CD	1:D:101:GLU:H	2.08	0.62
1:A:530:ASP:OD1	1:A:532:SER:HB3	2.00	0.61
1:A:70:LEU:HD22	1:A:70:LEU:N	2.14	0.61
1:B:208:LEU:O	1:B:212:ARG:HG2	2.00	0.61
1:C:345:VAL:HG13	1:C:372:THR:OG1	2.00	0.61
1:D:295:LYS:NZ	1:D:358:ILE:HG21	2.15	0.61
1:A:301:HIS:HB2	1:A:319:PHE:CD2	2.34	0.61
1:B:222:MET:HE2	1:B:291:LEU:HB2	1.82	0.61
1:C:193:THR:OG1	1:C:607:THR:HG22	1.99	0.61
1:C:259:VAL:HB	1:C:261:ARG:HH12	1.65	0.61
1:C:390:ILE:HG22	1:C:394:CYS:SG	2.40	0.61
1:D:261:ARG:HH12	1:D:271:HIS:HB3	1.65	0.61
1:D:349:LEU:HD23	1:D:369:THR:HG23	1.82	0.61
1:D:451:VAL:HA	1:D:470:LEU:O	1.99	0.61
1:A:349:LEU:HD23	1:A:369:THR:HG22	1.81	0.61
1:B:288:MET:CE	1:B:299:LEU:HD23	2.30	0.61
1:B:400:ALA:HB3	1:B:401:PRO:CD	2.30	0.61
1:C:297:ALA:H	1:C:358:ILE:HD11	1.65	0.61
1:C:389:LYS:HG2	1:C:485:VAL:HG21	1.81	0.61
1:D:263:PRO:HG2	1:D:265:LEU:CD1	2.31	0.61
1:B:227:MET:HE1	1:B:294:LEU:N	2.14	0.61
1:B:325:GLY:C	1:B:327:TRP:H	2.08	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:N	1:B:62:ILE:HD12	2.16	0.61
1:C:210:LEU:HD11	1:C:582:PHE:HE2	1.65	0.61
1:D:93:LYS:HA	1:D:93:LYS:HZ1	1.63	0.61
1:A:450:ASN:O	1:A:451:VAL:HB	1.99	0.61
1:C:546:SER:CB	1:C:547:ARG:HE	2.14	0.61
1:D:45:LEU:O	1:D:104:SER:HA	2.01	0.61
1:A:77:LYS:O	1:A:92:LEU:HD12	2.00	0.61
1:C:546:SER:HB3	1:C:547:ARG:HE	1.64	0.61
1:A:303:GLU:HB2	1:A:306:ILE:CD1	2.31	0.61
1:A:95:ARG:NH1	1:A:95:ARG:HB2	2.16	0.61
1:B:121:THR:HG23	1:B:128:VAL:HG13	1.82	0.61
1:C:548:SER:O	1:C:550:SER:N	2.33	0.61
1:D:557:LEU:HD12	1:D:596:HIS:CE1	2.36	0.61
1:B:531:THR:HG22	1:B:536:HIS:CD2	2.35	0.61
1:C:48:THR:HG21	1:C:103:LEU:HD12	1.82	0.61
1:D:70:LEU:HD13	1:D:117:TRP:CZ2	2.36	0.61
1:B:60:ILE:O	1:B:83:PRO:HD2	2.01	0.61
1:D:263:PRO:HG2	1:D:265:LEU:HD12	1.83	0.61
1:D:87:GLY:O	1:D:89:PRO:HD3	2.01	0.61
1:A:472:TRP:CE3	1:A:473:ILE:HG12	2.37	0.60
1:B:396:ASN:N	1:B:397:PRO:HD3	2.15	0.60
1:C:538:VAL:HG23	1:C:557:LEU:HD11	1.82	0.60
1:A:41:SER:O	1:A:110:SER:OG	2.19	0.60
1:B:93:LYS:CD	1:B:94:ASP:H	2.13	0.60
1:C:210:LEU:HD13	1:C:597:SER:CB	2.31	0.60
1:D:514:LEU:HD12	1:D:526:LEU:HB3	1.83	0.60
1:D:303:GLU:HG3	1:D:304:ASP:N	2.17	0.60
1:A:93:LYS:CD	1:A:94:ASP:H	2.15	0.60
1:A:95:ARG:HB2	1:A:95:ARG:CZ	2.32	0.60
1:B:455:THR:HB	1:B:514:LEU:HD22	1.84	0.60
1:A:212:ARG:HD3	1:C:201:MET:SD	2.42	0.60
1:A:270:PHE:CE1	1:A:599:MET:HE1	2.37	0.60
1:A:481:TYR:C	1:A:482:ARG:HG2	2.26	0.60
1:B:288:MET:HE1	1:B:299:LEU:HD23	1.82	0.60
1:D:377:ARG:HG3	1:D:377:ARG:NH1	2.16	0.60
1:C:388:GLY:O	1:C:391:GLN:HB3	2.01	0.60
1:D:261:ARG:NH1	1:D:261:ARG:CB	2.65	0.60
1:A:188:CYS:SG	1:A:549:PHE:HZ	2.25	0.60
1:C:252:TYR:HE1	1:C:279:PRO:HG3	1.66	0.60
1:C:358:ILE:HA	1:C:362:GLN:O	2.01	0.60
1:D:505:ASP:HB3	1:D:508:VAL:HG23	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:PHE:O	1:B:549:PHE:CD1	2.55	0.60
1:C:236:LYS:HB2	1:C:237:PRO:CD	2.32	0.60
1:C:384:GLN:HE22	1:C:490:ALA:CA	2.14	0.60
1:C:43:VAL:HG22	1:C:107:ILE:HB	1.83	0.60
1:B:202:SER:O	1:B:203:LEU:HD23	2.02	0.59
1:C:392:ALA:C	1:C:394:CYS:H	2.11	0.59
1:D:378:MET:CB	1:D:407:ILE:HG21	2.32	0.59
1:A:56:MET:HG2	1:A:57:ASN:N	2.17	0.59
1:A:261:ARG:O	1:A:263:PRO:HD3	2.02	0.59
1:A:46:PRO:O	1:A:48:THR:O	2.21	0.59
1:C:81:LEU:CD2	1:C:89:PRO:HB3	2.30	0.59
1:B:121:THR:CG2	1:B:128:VAL:HG13	2.33	0.59
1:C:546:SER:HB3	1:C:547:ARG:CZ	2.33	0.59
1:D:498:THR:HG22	1:D:499:TYR:N	2.17	0.59
1:A:507:ASP:HB3	1:A:532:SER:N	2.17	0.59
1:C:413:LEU:HD23	1:C:427:ILE:HB	1.83	0.59
1:D:514:LEU:CD1	1:D:526:LEU:HB3	2.33	0.59
1:D:520:GLN:H	1:D:520:GLN:HE21	1.51	0.59
1:A:488:LYS:O	1:A:489:GLU:HB2	2.03	0.59
1:C:542:VAL:HG21	1:C:551:TYR:CZ	2.38	0.59
1:C:91:TYR:C	1:C:93:LYS:H	2.07	0.59
1:B:346:ILE:HG23	1:B:369:THR:CG2	2.33	0.59
1:C:537:ALA:HA	1:C:557:LEU:HG	1.84	0.59
1:D:121:THR:HG23	1:D:128:VAL:CG1	2.31	0.59
1:A:38:GLN:HE21	1:D:422:GLU:HB3	1.68	0.58
1:C:369:THR:CG2	1:C:411:GLY:HA3	2.32	0.58
1:D:222:MET:CE	1:D:291:LEU:HB2	2.28	0.58
1:D:286:ASN:HD21	1:D:304:ASP:HB3	1.67	0.58
1:A:293:GLU:O	1:A:295:LYS:HG2	2.03	0.58
1:B:570:CYS:HB3	1:B:577:LEU:CD2	2.33	0.58
1:D:398:GLU:O	1:D:403:LYS:HE3	2.03	0.58
1:B:541:TYR:HB3	1:B:543:TYR:HE2	1.68	0.58
1:B:93:LYS:CG	1:B:94:ASP:H	2.16	0.58
1:C:132:CYS:SG	1:C:133:LEU:N	2.72	0.58
1:D:483:PHE:HZ	1:D:524:TYR:OH	1.87	0.58
1:D:580:ARG:HA	1:D:598:GLY:O	2.03	0.58
1:A:91:TYR:HB2	1:A:93:LYS:HG2	1.86	0.58
1:B:472:TRP:CZ3	1:B:473:ILE:HG13	2.39	0.58
1:A:272:MET:HE2	1:C:271:HIS:CE1	2.39	0.58
1:C:61:HIS:HB3	1:C:123:GLU:HB2	1.85	0.58
1:D:124:LYS:HG2	1:D:127:SER:HB2	1.83	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:HE1	1:A:351:LEU:HD22	1.85	0.58
1:B:325:GLY:C	1:B:327:TRP:N	2.61	0.58
1:A:224:SER:O	1:A:227:MET:HG2	2.04	0.58
1:B:140:GLN:HE22	1:C:422:GLU:HG2	1.68	0.58
1:C:540:TYR:HE1	1:C:568:VAL:CG2	2.17	0.58
1:D:472:TRP:CZ3	1:D:473:ILE:HB	2.39	0.58
1:A:299:LEU:HD21	1:A:425:ILE:HD13	1.85	0.57
1:A:437:HIS:CE1	1:A:459:MET:HB2	2.38	0.57
1:B:430:GLY:HA3	1:B:476:PHE:CE2	2.32	0.57
1:B:472:TRP:HE3	1:B:472:TRP:N	1.96	0.57
1:B:93:LYS:HD2	1:B:94:ASP:N	2.19	0.57
1:C:439:SER:CB	1:C:457:PRO:HG2	2.34	0.57
1:D:461:ASN:N	1:D:461:ASN:HD22	2.00	0.57
1:D:540:TYR:CE1	1:D:568:VAL:HG21	2.38	0.57
1:B:56:MET:HB3	1:B:101:GLU:HA	1.86	0.57
1:A:378:MET:CB	1:A:407:ILE:HG21	2.34	0.57
1:B:340:SER:CB	1:B:426:LYS:HA	2.34	0.57
1:D:520:GLN:HG2	1:D:521:ASP:N	2.19	0.57
1:A:320:GLN:HG3	1:A:336:TRP:CZ2	2.39	0.57
1:A:540:TYR:HE1	1:A:568:VAL:CG2	2.08	0.57
1:B:215:ASN:HB2	1:B:235:GLU:HB2	1.86	0.57
1:C:323:LYS:HB3	1:C:333:MET:HG2	1.87	0.57
1:D:499:TYR:CD2	1:D:501:PRO:HD3	2.40	0.57
1:B:318:SER:HB3	1:B:337:VAL:O	2.04	0.57
1:B:526:LEU:C	1:B:526:LEU:HD12	2.29	0.57
1:D:520:GLN:HG2	1:D:521:ASP:OD2	2.05	0.57
1:D:124:LYS:HE2	1:D:127:SER:CB	2.34	0.57
1:B:103:LEU:HD13	1:B:120:MET:CE	2.34	0.57
1:C:93:LYS:HD2	1:C:94:ASP:C	2.30	0.57
1:D:298:ALA:O	1:D:321:LEU:HD12	2.04	0.57
1:B:483:PHE:HZ	1:B:524:TYR:OH	1.87	0.57
1:D:236:LYS:HD3	1:D:252:TYR:CD2	2.40	0.57
1:D:66:MET:HE3	1:D:78:ILE:HD11	1.87	0.57
1:B:303:GLU:O	1:B:306:ILE:HD11	2.04	0.57
1:C:235:GLU:HA	1:C:250:SER:O	2.05	0.57
1:C:390:ILE:CG2	1:C:393:LEU:HB2	2.34	0.57
1:C:38:GLN:HG3	1:C:138:TYR:CE2	2.40	0.57
1:D:542:VAL:HG21	1:D:551:TYR:CZ	2.40	0.57
1:A:210:LEU:O	1:A:213:GLY:N	2.32	0.57
1:A:326:VAL:HG23	1:A:327:TRP:NE1	2.19	0.57
1:A:84:SER:O	1:A:85:GLU:CB	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:PHE:HB2	1:C:425:ILE:CD1	2.35	0.57
1:D:552:PHE:HE1	1:D:121:THR:HG1	1.52	0.57
1:A:216:VAL:HA	1:A:233:LEU:O	2.05	0.57
1:A:274:ASN:ND2	1:A:324:LEU:HB3	2.17	0.57
1:B:326:VAL:HG13	1:B:327:TRP:CD1	2.40	0.57
1:B:357:VAL:HG21	1:B:452:TYR:CE1	2.39	0.57
1:C:459:MET:HE3	1:C:462:LEU:HD12	1.86	0.57
1:D:293:GLU:OE1	1:D:360:ASP:N	2.38	0.57
1:B:557:LEU:HB3	1:B:559:ILE:HD13	1.85	0.56
1:C:540:TYR:HE1	1:C:568:VAL:HG21	1.70	0.56
1:C:259:VAL:HB	1:C:261:ARG:NH1	2.20	0.56
1:C:537:ALA:HB2	1:C:556:ARG:HA	1.87	0.56
1:C:81:LEU:HD22	1:C:82:ASP:H	1.70	0.56
1:B:459:MET:SD	1:B:459:MET:C	2.89	0.56
1:C:248:GLN:N	1:C:248:GLN:OE1	2.39	0.56
1:C:326:VAL:HG13	1:C:327:TRP:N	2.19	0.56
1:C:454:LEU:C	1:C:454:LEU:HD23	2.29	0.56
1:D:514:LEU:HD11	1:D:526:LEU:HD23	1.88	0.56
1:A:399:TRP:CZ3	1:A:435:ILE:HG22	2.41	0.56
1:B:458:PRO:HB2	1:B:511:SER:OG	2.05	0.56
1:B:89:PRO:HG2	1:B:91:TYR:HE2	1.69	0.56
1:C:262:ASN:HB2	1:C:573:TRP:HZ2	1.71	0.56
1:D:124:LYS:HE2	1:D:127:SER:HB2	1.87	0.56
1:B:541:TYR:HB3	1:B:543:TYR:CE2	2.39	0.56
1:B:134:HIS:CE1	1:B:136:LYS:NZ	2.74	0.56
1:B:100:LEU:HD13	1:B:100:LEU:O	2.06	0.56
1:C:349:LEU:HD23	1:C:369:THR:HG22	1.87	0.56
1:D:229:GLY:HA2	1:D:256:GLU:O	2.06	0.56
1:D:342:ASP:O	1:D:344:PRO:HD3	2.05	0.56
1:D:34:LYS:HE3	1:D:134:HIS:HD2	1.70	0.56
1:B:378:MET:HB2	1:B:407:ILE:HD13	1.88	0.56
1:B:418:SER:O	1:B:419:LEU:HD12	2.06	0.56
1:D:565:GLU:HB3	1:D:584:VAL:HB	1.87	0.56
1:C:349:LEU:CD2	1:C:369:THR:HG22	2.36	0.55
1:C:375:LYS:O	1:C:379:GLU:HB3	2.06	0.55
1:D:253:ARG:HH21	1:D:285:SER:CB	2.18	0.55
1:A:500:LEU:C	1:A:502:ALA:H	2.15	0.55
1:A:301:HIS:ND1	1:A:302:GLY:N	2.55	0.55
1:A:358:ILE:HG12	1:A:363:ALA:HB2	1.89	0.55
1:A:39:LEU:HB2	1:A:138:TYR:O	2.06	0.55
1:B:61:HIS:HE1	1:B:63:VAL:HG22	1.68	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:SER:HB3	1:C:547:ARG:NE	2.21	0.55
1:D:355:ARG:HB2	1:D:442:ASP:HB3	1.87	0.55
1:D:559:ILE:HG12	1:D:560:LYS:N	2.21	0.55
1:A:202:SER:OG	1:A:203:LEU:N	2.39	0.55
1:B:140:GLN:HE21	1:C:422:GLU:H	1.55	0.55
1:C:36:VAL:HA	1:C:136:LYS:O	2.06	0.55
1:C:82:ASP:CG	1:C:84:SER:HB3	2.31	0.55
1:D:444:TYR:HB2	1:D:453:TRP:HB2	1.89	0.55
1:D:493:ASP:HB2	1:D:495:HIS:NE2	2.21	0.55
1:D:200:ASN:H	1:D:200:ASN:HD22	1.52	0.55
1:A:337:VAL:HG12	1:A:425:ILE:HG13	1.88	0.55
1:C:464:LEU:HD22	1:C:498:THR:HB	1.88	0.55
1:C:139:GLU:OE2	1:C:139:GLU:N	2.40	0.55
1:D:81:LEU:HD23	1:D:82:ASP:N	2.22	0.55
1:C:410:TYR:O	1:C:429:SER:HA	2.07	0.55
1:C:34:LYS:HD2	1:C:34:LYS:N	2.22	0.55
1:D:461:ASN:O	1:D:504:VAL:HG21	2.06	0.55
1:B:475:ARG:O	1:B:476:PHE:CB	2.54	0.55
1:D:450:ASN:O	1:D:471:GLU:HA	2.07	0.55
1:D:515:VAL:HG13	1:D:525:VAL:HG23	1.89	0.55
1:D:200:ASN:H	1:D:200:ASN:ND2	2.05	0.55
1:D:64:VAL:HB	1:D:79:VAL:HG13	1.88	0.55
1:B:389:LYS:HG3	1:B:390:ILE:N	2.21	0.55
1:B:472:TRP:N	1:B:472:TRP:CE3	2.75	0.55
1:D:503:GLU:HG2	1:D:93:LYS:CD	2.37	0.55
1:B:517:LEU:HB2	1:B:523:GLN:HG3	1.89	0.54
1:D:206:LEU:HD22	1:D:210:LEU:HD11	1.89	0.54
1:D:289:VAL:HG13	1:D:296:LEU:CD1	2.38	0.54
1:D:124:LYS:HE2	1:D:127:SER:OG	2.06	0.54
1:A:378:MET:HB3	1:A:407:ILE:HD13	1.89	0.54
1:A:437:HIS:ND1	1:A:459:MET:HB2	2.21	0.54
1:B:540:TYR:HE1	1:B:568:VAL:HG21	1.72	0.54
1:C:321:LEU:N	1:C:335:SER:O	2.31	0.54
1:C:410:TYR:HD2	1:C:454:LEU:HD11	1.73	0.54
1:D:251:MET:HE2	1:D:283:ASP:HB3	1.89	0.54
1:D:295:LYS:HZ2	1:D:358:ILE:HG21	1.71	0.54
1:A:446:SER:OG	1:A:451:VAL:HG13	2.07	0.54
1:B:589:GLU:HG2	1:B:590:SER:H	1.72	0.54
1:C:288:MET:HB2	1:C:365:TRP:NE1	2.23	0.54
1:D:376:LEU:HD23	1:D:376:LEU:O	2.08	0.54
1:D:383:GLN:HA	1:D:386:CYS:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HD21	1:A:425:ILE:CD1	2.38	0.54
1:A:459:MET:HA	1:A:459:MET:CE	2.38	0.54
1:B:217:SER:O	1:B:218:SER:HB2	2.06	0.54
1:B:542:VAL:O	1:B:550:SER:HA	2.07	0.54
1:B:40:GLY:HA2	1:B:110:SER:O	2.08	0.54
1:C:198:PHE:CE1	1:C:600:VAL:HB	2.43	0.54
1:D:219:ILE:HD12	1:D:219:ILE:N	2.21	0.54
1:C:215:ASN:O	1:C:234:VAL:HA	2.08	0.54
1:C:461:ASN:HB3	1:C:508:VAL:HG13	1.89	0.54
1:D:44:LEU:HD11	1:D:104:SER:HB2	1.88	0.54
1:D:483:PHE:HZ	1:D:524:TYR:HH	1.55	0.54
1:B:255:PHE:HD1	1:B:276:LEU:HD22	1.73	0.54
1:B:132:CYS:SG	1:B:133:LEU:N	2.81	0.54
1:C:222:MET:HE2	1:C:291:LEU:HB2	1.90	0.54
1:C:485:VAL:HG23	1:C:485:VAL:O	2.08	0.54
1:A:322:VAL:HG12	1:A:324:LEU:CD1	2.37	0.54
1:A:121:THR:HG23	1:A:128:VAL:HG13	1.89	0.54
1:D:345:VAL:HG23	1:D:372:THR:OG1	2.08	0.54
1:D:394:CYS:O	1:D:397:PRO:HD3	2.08	0.54
1:D:93:LYS:HA	1:D:93:LYS:HZ2	1.73	0.54
1:A:558:PRO:HG2	1:A:559:ILE:HG23	1.89	0.54
1:A:68:LYS:H	1:A:68:LYS:HD2	1.72	0.54
1:C:93:LYS:HD2	1:C:94:ASP:H	1.69	0.54
1:D:496:ALA:HB1	1:D:497:PRO:HD2	1.89	0.54
1:D:530:ASP:OD2	1:D:533:ARG:NH1	2.40	0.54
1:B:208:LEU:HD12	1:B:212:ARG:HD3	1.89	0.54
1:B:514:LEU:C	1:B:514:LEU:HD23	2.33	0.54
1:B:499:TYR:CZ	1:B:501:PRO:HB3	2.43	0.53
1:C:125:ASN:OD1	1:C:126:ILE:HG13	2.07	0.53
1:D:537:ALA:HB2	1:D:556:ARG:HA	1.89	0.53
1:D:92:LEU:HD23	1:D:92:LEU:H	1.72	0.53
1:A:261:ARG:C	1:A:263:PRO:HD3	2.33	0.53
1:B:385:ALA:HB2	1:B:487:ILE:HG13	1.91	0.53
1:B:65:THR:HB	1:B:75:GLU:HG3	1.89	0.53
1:C:341:THR:HA	1:C:427:ILE:HG23	1.89	0.53
1:C:323:LYS:HD3	1:C:333:MET:HE3	1.91	0.53
1:D:219:ILE:O	1:D:567:GLN:HG3	2.09	0.53
1:D:377:ARG:O	1:D:377:ARG:HD3	2.09	0.53
1:A:47:LEU:HA	1:A:133:LEU:HD12	1.91	0.53
1:B:140:GLN:NE2	1:C:422:GLU:HG2	2.22	0.53
1:A:438:GLY:O	1:A:440:GLY:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:HD21	1:C:498:THR:HB	1.90	0.53
1:C:82:ASP:C	1:C:84:SER:H	2.17	0.53
1:D:265:LEU:HD12	1:D:269:VAL:HG21	1.89	0.53
1:D:329:SER:HB2	1:D:330:PRO:HD2	1.90	0.53
1:B:471:GLU:O	1:B:476:PHE:HA	2.09	0.53
1:C:323:LYS:CD	1:C:333:MET:HE3	2.39	0.53
1:D:580:ARG:NH1	1:D:597:SER:OG	2.42	0.53
1:A:455:THR:CG2	1:A:516:ILE:HD11	2.38	0.53
1:A:519:GLY:O	1:B:520:GLN:HG2	2.08	0.53
1:B:464:LEU:HD11	1:B:526:LEU:HD21	1.90	0.53
1:A:227:MET:HE1	1:A:294:LEU:H	1.73	0.53
1:A:268:PRO:HD3	1:A:573:TRP:CE3	2.44	0.53
1:B:308:ILE:HG23	1:B:341:THR:HG22	1.91	0.53
1:B:437:HIS:CD2	1:B:459:MET:HB2	2.44	0.53
1:D:64:VAL:HB	1:D:79:VAL:CG1	2.39	0.53
1:B:36:VAL:O	1:B:37:GLN:HG2	2.09	0.53
1:B:255:PHE:CZ	1:B:322:VAL:HG21	2.44	0.52
1:B:262:ASN:HB2	1:B:573:TRP:HZ2	1.74	0.52
1:B:507:ASP:O	1:B:530:ASP:HA	2.10	0.52
1:C:219:ILE:HG21	1:C:582:PHE:CG	2.44	0.52
1:D:461:ASN:O	1:D:462:LEU:HD23	2.08	0.52
1:A:533:ARG:NH1	1:A:554:PRO:HB3	2.24	0.52
1:D:231:THR:HG22	1:D:289:VAL:CG2	2.39	0.52
1:D:488:LYS:HG3	1:D:489:GLU:HG2	1.92	0.52
1:B:277:GLU:O	1:B:278:GLN:HG3	2.09	0.52
1:B:392:ALA:HA	1:B:395:GLU:CD	2.35	0.52
1:C:200:ASN:OD1	1:C:200:ASN:N	2.41	0.52
1:C:236:LYS:C	1:C:249:LEU:HB3	2.34	0.52
1:C:548:SER:O	1:C:549:PHE:C	2.51	0.52
1:D:537:ALA:CB	1:D:556:ARG:HA	2.40	0.52
1:A:384:GLN:HG3	1:A:490:ALA:HB2	1.90	0.52
1:D:437:HIS:O	1:D:459:MET:SD	2.68	0.52
1:C:91:TYR:HB3	1:C:93:LYS:HB3	1.90	0.52
1:D:280:VAL:HG12	1:D:282:ASN:H	1.73	0.52
1:A:222:MET:SD	1:A:355:ARG:HG2	2.50	0.52
1:B:120:MET:HE3	1:B:122:LEU:HD21	1.92	0.52
1:D:472:TRP:CE3	1:D:473:ILE:HB	2.44	0.52
1:A:437:HIS:C	1:A:439:SER:H	2.18	0.52
1:A:52:ILE:O	1:A:53:ASN:HB3	2.10	0.52
1:A:123:GLU:HG2	1:A:128:VAL:HG22	1.91	0.52
1:B:262:ASN:HB2	1:B:573:TRP:CZ2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:TYR:CD1	1:B:478:VAL:HG11	2.45	0.52
1:C:589:GLU:C	1:C:591:GLY:H	2.17	0.52
1:A:215:ASN:O	1:A:234:VAL:HA	2.08	0.52
1:B:389:LYS:HG3	1:B:390:ILE:HG23	1.91	0.52
1:B:140:GLN:NE2	1:C:422:GLU:H	2.08	0.52
1:A:273:THR:HB	1:A:326:VAL:O	2.10	0.52
1:A:430:GLY:HA3	1:A:476:PHE:HE2	1.73	0.52
1:A:94:ASP:HB3	1:A:95:ARG:HH11	1.75	0.52
1:A:132:CYS:O	1:A:133:LEU:HB2	2.09	0.52
1:B:251:MET:SD	1:B:283:ASP:HB3	2.50	0.52
1:B:413:LEU:HD12	1:B:427:ILE:CD1	2.40	0.52
1:B:73:SER:OG	1:B:74:VAL:N	2.41	0.52
1:C:229:GLY:HA3	1:C:296:LEU:HD12	1.92	0.52
1:D:93:LYS:HG3	1:D:94:ASP:N	2.25	0.52
1:A:188:CYS:SG	1:A:549:PHE:CZ	3.04	0.52
1:A:393:LEU:HD21	1:A:436:THR:CB	2.40	0.52
1:B:210:LEU:O	1:B:213:GLY:N	2.36	0.52
1:C:363:ALA:O	1:C:414:SER:HA	2.09	0.52
1:A:519:GLY:C	1:A:521:ASP:H	2.17	0.51
1:A:38:GLN:OE1	1:A:38:GLN:HA	2.10	0.51
1:B:264:GLY:C	1:B:265:LEU:HD12	2.35	0.51
1:B:514:LEU:HD23	1:B:514:LEU:O	2.10	0.51
1:D:319:PHE:HB2	1:D:425:ILE:CD1	2.39	0.51
1:A:551:TYR:CD2	1:A:552:PHE:N	2.78	0.51
1:B:294:LEU:HB3	1:B:326:VAL:HG12	1.91	0.51
1:D:227:MET:HE1	1:D:295:LYS:O	2.11	0.51
1:A:71:GLU:O	1:A:72:ASN:CB	2.57	0.51
1:A:101:GLU:H	1:A:101:GLU:CD	2.18	0.51
1:D:577:LEU:C	1:D:577:LEU:HD22	2.35	0.51
1:D:95:ARG:H	1:D:95:ARG:HE	1.58	0.51
1:A:193:THR:HG22	1:A:129:GLN:HG3	1.91	0.51
1:A:388:GLY:O	1:A:391:GLN:HB2	2.11	0.51
1:C:210:LEU:HD13	1:C:597:SER:HB3	1.92	0.51
1:C:49:HIS:O	1:C:50:GLU:HG3	2.11	0.51
1:D:206:LEU:HD22	1:D:210:LEU:CD1	2.40	0.51
1:B:475:ARG:HH12	1:B:477:LYS:HD3	1.72	0.51
1:D:206:LEU:CD2	1:D:210:LEU:HG	2.40	0.51
1:D:389:LYS:C	1:D:391:GLN:H	2.19	0.51
1:A:556:ARG:NH2	1:A:125:ASN:O	2.44	0.51
1:A:580:ARG:HB3	1:A:599:MET:CE	2.38	0.51
1:B:238:ASN:O	1:B:239:LEU:HB2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:HIS:CG	1:C:306:ILE:HD11	2.46	0.51
1:C:461:ASN:ND2	1:C:462:LEU:HD23	2.26	0.51
1:D:112:LYS:HB2	1:D:112:LYS:NZ	2.25	0.51
1:A:318:SER:HB3	1:A:337:VAL:O	2.11	0.51
1:B:378:MET:CB	1:B:407:ILE:HD13	2.40	0.51
1:B:458:PRO:HG3	1:B:465:GLY:N	2.23	0.51
1:C:121:THR:HG22	1:C:128:VAL:CG2	2.41	0.51
1:A:79:VAL:O	1:A:79:VAL:HG13	2.11	0.51
1:C:50:GLU:O	1:C:51:ARG:C	2.54	0.51
1:C:135:LEU:HD23	1:C:135:LEU:C	2.35	0.51
1:D:221:THR:HG22	1:D:230:GLY:HA3	1.93	0.51
1:B:374:ASP:C	1:B:376:LEU:H	2.19	0.51
1:B:37:GLN:O	1:B:137:LEU:HA	2.11	0.51
1:B:51:ARG:C	1:B:53:ASN:H	2.19	0.51
1:C:541:TYR:CE1	1:C:552:PHE:CB	2.94	0.51
1:D:261:ARG:HH12	1:D:271:HIS:CB	2.23	0.51
1:D:38:GLN:HB3	1:D:41:SER:HB3	1.93	0.51
1:A:533:ARG:NH1	1:A:123:GLU:OE1	2.44	0.51
1:A:580:ARG:CG	1:A:580:ARG:NH1	2.74	0.51
1:B:585:LEU:HD12	1:B:585:LEU:N	2.26	0.51
1:B:134:HIS:CE1	1:B:136:LYS:HZ2	2.29	0.51
1:C:293:GLU:HB2	1:C:295:LYS:HE2	1.92	0.51
1:C:391:GLN:HG2	1:C:392:ALA:N	2.25	0.51
1:C:451:VAL:CG1	1:C:469:THR:HB	2.41	0.51
1:C:472:TRP:CZ3	1:C:473:ILE:HD13	2.46	0.51
1:D:577:LEU:HD22	1:D:578:TRP:N	2.25	0.51
1:B:299:LEU:HD21	1:B:425:ILE:HD13	1.93	0.50
1:B:319:PHE:HB2	1:B:425:ILE:HD11	1.93	0.50
1:C:194:ILE:HA	1:C:603:GLY:O	2.11	0.50
1:C:421:VAL:O	1:C:422:GLU:C	2.53	0.50
1:C:437:HIS:ND1	1:C:459:MET:HG2	2.26	0.50
1:C:589:GLU:O	1:C:591:GLY:N	2.43	0.50
1:D:510:LEU:HD12	1:D:511:SER:H	1.76	0.50
1:B:354:HIS:ND1	1:B:367:VAL:HG12	2.26	0.50
1:B:221:THR:HG22	1:B:230:GLY:HA3	1.93	0.50
1:B:259:VAL:HG12	1:B:260:ILE:N	2.26	0.50
1:B:61:HIS:C	1:B:62:ILE:HD12	2.37	0.50
1:C:293:GLU:HB3	1:C:295:LYS:HE2	1.93	0.50
1:A:437:HIS:O	1:A:439:SER:N	2.45	0.50
1:A:565:GLU:HB3	1:A:584:VAL:HB	1.94	0.50
1:C:461:ASN:C	1:C:461:ASN:ND2	2.67	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:LYS:C	1:C:489:GLU:HG2	2.37	0.50
1:D:48:THR:HG21	1:D:103:LEU:HD13	1.93	0.50
1:C:36:VAL:C	1:C:37:GLN:HE21	2.19	0.50
1:A:449:ASN:O	1:A:472:TRP:HH2	1.94	0.50
1:C:369:THR:HG23	1:C:411:GLY:HA3	1.91	0.50
1:A:371:ARG:HD2	1:A:429:SER:HB2	1.93	0.50
1:C:236:LYS:CB	1:C:237:PRO:CD	2.90	0.50
1:C:453:TRP:HB3	1:C:516:ILE:HD12	1.93	0.50
1:D:219:ILE:HG21	1:D:582:PHE:CD1	2.47	0.50
1:D:378:MET:HG3	1:D:431:PHE:CE2	2.47	0.50
1:A:499:TYR:CZ	1:A:501:PRO:HB3	2.45	0.50
1:A:50:GLU:HG2	1:A:52:ILE:CG2	2.41	0.50
1:B:299:LEU:HD11	1:B:425:ILE:HD11	1.94	0.50
1:B:500:LEU:CD2	1:B:502:ALA:HB3	2.42	0.50
1:B:60:ILE:HD12	1:B:124:LYS:HA	1.92	0.50
1:D:464:LEU:CG	1:D:465:GLY:H	2.23	0.50
1:A:458:PRO:HB2	1:A:511:SER:CB	2.41	0.50
1:A:485:VAL:O	1:A:495:HIS:HB3	2.12	0.50
1:B:282:ASN:OD1	1:B:284:LEU:HB2	2.12	0.50
1:B:337:VAL:CG1	1:B:423:LEU:HB3	2.42	0.50
1:C:201:MET:HE1	1:C:265:LEU:HB3	1.94	0.50
1:D:441:MET:HA	1:D:455:THR:O	2.12	0.50
1:A:93:LYS:HD2	1:A:94:ASP:CA	2.43	0.49
1:B:47:LEU:HD13	1:B:120:MET:HB2	1.93	0.49
1:B:51:ARG:O	1:B:53:ASN:N	2.45	0.49
1:D:306:ILE:N	1:D:306:ILE:CD1	2.75	0.49
1:D:326:VAL:HG13	1:D:327:TRP:N	2.28	0.49
1:B:453:TRP:CE2	1:B:522:LEU:HD13	2.47	0.49
1:D:415:VAL:CG1	1:D:425:ILE:HA	2.42	0.49
1:A:466:VAL:CG1	1:A:468:ASN:HD21	2.26	0.49
1:B:326:VAL:HG22	1:B:326:VAL:O	2.12	0.49
1:D:354:HIS:ND1	1:D:367:VAL:HG12	2.26	0.49
1:D:456:ILE:HG22	1:D:459:MET:HE2	1.94	0.49
1:D:547:ARG:HG3	1:D:549:PHE:H	1.76	0.49
1:C:459:MET:SD	1:C:460:LYS:HB2	2.53	0.49
1:A:320:GLN:HB2	1:A:336:TRP:CH2	2.47	0.49
1:B:308:ILE:N	1:B:308:ILE:HD12	2.27	0.49
1:B:85:GLU:HG3	1:B:87:GLY:H	1.77	0.49
1:C:367:VAL:HG13	1:C:368:PRO:HD2	1.93	0.49
1:D:481:TYR:CD2	1:D:482:ARG:HG2	2.47	0.49
1:A:233:LEU:HD23	1:A:253:ARG:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:PRO:HB3	1:D:465:GLY:N	2.28	0.49
1:D:135:LEU:HD12	1:D:136:LYS:H	1.76	0.49
1:B:540:TYR:HE1	1:B:568:VAL:CG2	2.25	0.49
1:B:280:VAL:HG12	1:B:282:ASN:H	1.77	0.49
1:B:293:GLU:O	1:B:295:LYS:HG2	2.13	0.49
1:C:287:CYS:HA	1:C:299:LEU:O	2.13	0.49
1:C:509:LYS:HB2	1:C:563:PRO:HG3	1.94	0.49
1:D:295:LYS:HA	1:D:325:GLY:HA2	1.94	0.49
1:D:503:GLU:HG2	1:D:93:LYS:HD2	1.93	0.49
1:D:523:GLN:O	1:D:524:TYR:HB3	2.12	0.49
1:C:227:MET:HB2	1:C:258:GLY:O	2.13	0.49
1:C:472:TRP:CD1	1:C:472:TRP:N	2.81	0.49
1:C:541:TYR:CE1	1:C:552:PHE:HB3	2.48	0.49
1:D:231:THR:HG21	1:D:287:CYS:HB2	1.95	0.49
1:A:192:THR:HG22	1:A:606:CYS:SG	2.53	0.48
1:B:559:ILE:HG12	1:B:560:LYS:N	2.28	0.48
1:C:206:LEU:CD2	1:C:210:LEU:HG	2.42	0.48
1:C:255:PHE:O	1:C:275:TYR:HB2	2.13	0.48
1:D:464:LEU:HG	1:D:465:GLY:N	2.23	0.48
1:B:306:ILE:HD12	1:B:306:ILE:N	2.27	0.48
1:C:99:TYR:HB3	1:C:101:GLU:HG2	1.95	0.48
1:D:211:GLY:C	1:D:213:GLY:N	2.68	0.48
1:D:547:ARG:CG	1:D:548:SER:H	2.26	0.48
1:A:257:VAL:HG13	1:A:274:ASN:HB3	1.94	0.48
1:A:337:VAL:HG11	1:A:425:ILE:HG13	1.94	0.48
1:B:562:VAL:CB	1:B:586:ALA:HB3	2.39	0.48
1:C:230:GLY:HA2	1:C:289:VAL:HG11	1.95	0.48
1:C:68:LYS:HD3	1:C:113:LYS:O	2.12	0.48
1:D:399:TRP:O	1:D:403:LYS:HG3	2.14	0.48
1:D:75:GLU:OE2	1:D:130:ARG:NH2	2.41	0.48
1:A:466:VAL:CG1	1:A:468:ASN:ND2	2.76	0.48
1:A:52:ILE:O	1:A:52:ILE:HG12	2.13	0.48
1:B:513:ASN:OD1	1:B:568:VAL:HG12	2.13	0.48
1:B:540:TYR:O	1:B:552:PHE:HA	2.14	0.48
1:B:95:ARG:HG3	1:B:95:ARG:NH1	2.22	0.48
1:C:38:GLN:O	1:C:41:SER:OG	2.32	0.48
1:A:222:MET:HB3	1:A:355:ARG:CD	2.41	0.48
1:A:36:VAL:C	1:A:37:GLN:HG2	2.38	0.48
1:C:541:TYR:CD1	1:C:552:PHE:HB3	2.49	0.48
1:D:253:ARG:HH11	1:D:253:ARG:HG3	1.78	0.48
1:D:307:THR:HA	1:D:348:ARG:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TYR:C	1:A:312:GLY:H	2.22	0.48
1:A:520:GLN:O	1:A:520:GLN:CG	2.61	0.48
1:A:580:ARG:HB2	1:A:580:ARG:CZ	2.44	0.48
1:A:95:ARG:HH11	1:A:95:ARG:H	1.62	0.48
1:B:206:LEU:HD13	1:B:232:TYR:CD1	2.49	0.48
1:C:480:PRO:HB2	1:C:484:THR:HG21	1.95	0.48
1:D:321:LEU:N	1:D:335:SER:O	2.36	0.48
1:B:263:PRO:HB2	1:B:265:LEU:HD13	1.96	0.48
1:B:38:GLN:HG3	1:C:422:GLU:HB3	1.96	0.48
1:C:210:LEU:HD11	1:C:582:PHE:CE2	2.48	0.48
1:C:249:LEU:HD22	1:C:249:LEU:H	1.78	0.48
1:C:363:ALA:HB3	1:C:415:VAL:HG23	1.94	0.48
1:C:374:ASP:HB2	1:C:407:ILE:HB	1.95	0.48
1:C:37:GLN:HE21	1:C:37:GLN:CA	2.27	0.48
1:D:332:ASP:O	1:D:333:MET:HB3	2.13	0.48
1:A:399:TRP:CD1	1:A:401:PRO:HD2	2.49	0.48
1:B:441:MET:HE2	1:B:456:ILE:HD11	1.96	0.48
1:B:43:VAL:HG21	1:B:135:LEU:HD21	1.95	0.48
1:D:194:ILE:N	1:D:194:ILE:CD1	2.77	0.48
1:A:303:GLU:HB2	1:A:306:ILE:HD13	1.95	0.48
1:A:91:TYR:CB	1:A:93:LYS:HB3	2.42	0.48
1:A:135:LEU:HG	1:A:136:LYS:N	2.28	0.48
1:B:301:HIS:ND1	1:B:302:GLY:N	2.62	0.48
1:B:374:ASP:HB2	1:B:407:ILE:HB	1.96	0.48
1:B:533:ARG:HG3	1:B:533:ARG:HH11	1.79	0.48
1:D:198:PHE:CE1	1:D:600:VAL:HB	2.49	0.48
1:D:255:PHE:O	1:D:275:TYR:HA	2.14	0.48
1:D:280:VAL:HG12	1:D:281:SER:N	2.29	0.48
1:A:515:VAL:HG12	1:A:525:VAL:HB	1.96	0.48
1:A:55:SER:HB3	1:A:57:ASN:HD21	1.79	0.48
1:B:399:TRP:NE1	1:B:401:PRO:HD2	2.28	0.48
1:B:93:LYS:HB2	1:B:96:TYR:HD1	1.78	0.48
1:C:48:THR:HG22	1:C:103:LEU:HB2	1.95	0.48
1:D:482:ARG:HD2	1:D:72:ASN:HD21	1.79	0.48
1:C:39:LEU:C	1:C:41:SER:H	2.22	0.47
1:D:559:ILE:CG1	1:D:560:LYS:N	2.76	0.47
1:D:59:SER:HB2	1:D:123:GLU:O	2.14	0.47
1:A:309:PRO:HB2	1:A:341:THR:CG2	2.43	0.47
1:B:48:THR:C	1:B:50:GLU:H	2.20	0.47
1:B:91:TYR:CB	1:B:93:LYS:HB3	2.41	0.47
1:C:458:PRO:HD2	1:C:511:SER:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ILE:HD13	1:B:348:ARG:HA	1.95	0.47
1:D:467:ILE:HD12	1:D:483:PHE:HE2	1.79	0.47
1:A:510:LEU:O	1:A:528:THR:HA	2.14	0.47
1:B:37:GLN:HB2	1:B:137:LEU:HD23	1.97	0.47
1:B:47:LEU:HA	1:B:133:LEU:HD12	1.97	0.47
1:C:374:ASP:CG	1:C:406:ARG:HE	2.22	0.47
1:C:461:ASN:HD22	1:C:462:LEU:N	2.11	0.47
1:D:514:LEU:HD13	1:D:526:LEU:HD23	1.96	0.47
1:A:80:SER:O	1:A:81:LEU:HB2	2.14	0.47
1:C:390:ILE:CG2	1:C:394:CYS:SG	3.03	0.47
1:C:37:GLN:O	1:C:137:LEU:HA	2.15	0.47
1:A:125:ASN:OD1	1:A:126:ILE:N	2.48	0.47
1:C:219:ILE:HG21	1:C:582:PHE:CD2	2.50	0.47
1:C:288:MET:HB3	1:C:354:HIS:HB2	1.95	0.47
1:C:480:PRO:CB	1:C:484:THR:HG21	2.44	0.47
1:D:202:SER:O	1:D:203:LEU:HD23	2.14	0.47
1:D:537:ALA:HA	1:D:557:LEU:CD2	2.41	0.47
1:D:543:TYR:C	1:D:545:PRO:HD3	2.40	0.47
1:D:552:PHE:HE1	1:D:121:THR:OG1	1.97	0.47
1:A:472:TRP:CZ3	1:A:473:ILE:HG12	2.49	0.47
1:A:81:LEU:C	1:A:81:LEU:HD23	2.39	0.47
1:A:139:GLU:OE2	1:A:139:GLU:N	2.47	0.47
1:B:206:LEU:HD13	1:B:232:TYR:CG	2.49	0.47
1:B:294:LEU:N	1:B:294:LEU:HD22	2.29	0.47
1:C:209:TYR:O	1:C:210:LEU:C	2.56	0.47
1:C:369:THR:HG21	1:C:411:GLY:HA3	1.96	0.47
1:C:384:GLN:HE22	1:C:490:ALA:CB	2.28	0.47
1:C:531:THR:HG22	1:C:536:HIS:CG	2.48	0.47
1:C:569:GLU:O	1:C:569:GLU:HG3	2.15	0.47
1:C:91:TYR:HB3	1:C:93:LYS:HG2	1.95	0.47
1:D:261:ARG:HB2	1:D:261:ARG:CZ	2.45	0.47
1:D:347:ASP:H	1:D:371:ARG:HA	1.80	0.47
1:A:255:PHE:CZ	1:A:322:VAL:HG21	2.49	0.47
1:B:339:LEU:HD12	1:B:425:ILE:HB	1.95	0.47
1:B:91:TYR:C	1:B:93:LYS:H	2.21	0.47
1:C:99:TYR:O	1:C:100:LEU:C	2.58	0.47
1:A:524:TYR:N	1:A:524:TYR:CD2	2.83	0.47
1:C:522:LEU:HD12	1:C:523:GLN:N	2.29	0.47
1:D:374:ASP:HB3	1:D:407:ILE:HG12	1.97	0.47
1:D:564:ILE:HD12	1:D:564:ILE:C	2.40	0.47
1:D:600:VAL:HG13	1:D:602:MET:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:OE2	1:A:359:ALA:HA	2.15	0.47
1:A:475:ARG:O	1:A:476:PHE:C	2.58	0.47
1:A:517:LEU:HD11	1:A:525:VAL:HG23	1.97	0.47
1:B:471:GLU:OE2	1:B:477:LYS:O	2.32	0.47
1:C:81:LEU:HD22	1:C:82:ASP:N	2.30	0.47
1:A:569:GLU:OE2	1:A:582:PHE:HE1	1.97	0.46
1:A:98:PHE:HZ	1:A:103:LEU:HD22	1.79	0.46
1:D:261:ARG:HH11	1:D:261:ARG:HB3	1.80	0.46
1:D:324:LEU:HD23	1:D:332:ASP:HB3	1.96	0.46
1:D:501:PRO:O	1:D:504:VAL:HG12	2.15	0.46
1:B:77:LYS:NZ	1:B:80:SER:HB2	2.30	0.46
1:B:92:LEU:N	1:B:92:LEU:HD23	2.31	0.46
1:C:329:SER:OG	1:C:331:THR:HG23	2.14	0.46
1:C:540:TYR:CE1	1:C:568:VAL:HG21	2.50	0.46
1:D:228:TYR:CE1	1:D:258:GLY:HA3	2.51	0.46
1:A:299:LEU:CD1	1:A:321:LEU:HD13	2.46	0.46
1:C:35:ILE:HD13	1:C:45:LEU:HD23	1.97	0.46
1:D:288:MET:HE3	1:D:299:LEU:HB3	1.97	0.46
1:D:293:GLU:O	1:D:295:LYS:HE3	2.14	0.46
1:D:410:TYR:CE1	1:D:435:ILE:HD11	2.50	0.46
1:D:419:LEU:HD21	1:D:423:LEU:HD11	1.97	0.46
1:D:498:THR:HG22	1:D:499:TYR:H	1.80	0.46
1:D:36:VAL:HG22	1:D:136:LYS:HB3	1.97	0.46
1:D:43:VAL:HG22	1:D:45:LEU:CD1	2.45	0.46
1:A:38:GLN:NE2	1:D:422:GLU:HB3	2.31	0.46
1:B:126:ILE:O	1:B:126:ILE:HG13	2.15	0.46
1:D:514:LEU:HD12	1:D:514:LEU:HA	1.74	0.46
1:D:569:GLU:O	1:D:569:GLU:HG3	2.15	0.46
1:A:231:THR:OG1	1:A:253:ARG:HD2	2.16	0.46
1:A:507:ASP:OD1	1:A:90:ARG:NH1	2.47	0.46
1:A:38:GLN:HG3	1:D:422:GLU:HB3	1.98	0.46
1:B:36:VAL:C	1:B:37:GLN:HG2	2.40	0.46
1:B:52:ILE:HD13	1:C:282:ASN:OD1	2.16	0.46
1:D:538:VAL:HG21	1:D:581:HIS:CD2	2.50	0.46
1:D:556:ARG:HG3	1:D:556:ARG:HH21	1.81	0.46
1:D:39:LEU:HB2	1:D:138:TYR:O	2.16	0.46
1:A:230:GLY:HA2	1:A:289:VAL:HG11	1.98	0.46
1:A:318:SER:HB3	1:A:337:VAL:C	2.40	0.46
1:A:377:ARG:HG2	1:A:377:ARG:HH11	1.80	0.46
1:A:415:VAL:CG1	1:A:425:ILE:HG12	2.46	0.46
1:A:47:LEU:HD21	1:A:105:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:HH11	1:A:95:ARG:N	2.14	0.46
1:B:222:MET:HB3	1:B:355:ARG:HD3	1.98	0.46
1:C:107:ILE:HD11	1:C:118:TYR:HE2	1.78	0.46
1:D:521:ASP:HB2	1:D:546:SER:CB	2.44	0.46
1:A:45:LEU:HD13	1:A:133:LEU:HD13	1.98	0.46
1:B:262:ASN:C	1:B:264:GLY:H	2.24	0.46
1:C:121:THR:HG22	1:C:128:VAL:HG22	1.98	0.46
1:C:124:LYS:O	1:C:125:ASN:C	2.59	0.46
1:D:504:VAL:HG13	1:D:504:VAL:O	2.16	0.46
1:D:545:PRO:C	1:D:547:ARG:N	2.67	0.46
1:D:35:ILE:HG12	1:D:133:LEU:HD22	1.97	0.46
1:B:473:ILE:HB	1:B:474:PRO:CD	2.37	0.46
1:C:543:TYR:OH	1:C:75:GLU:HB2	2.16	0.46
1:A:93:LYS:HD2	1:A:94:ASP:O	2.15	0.46
1:C:236:LYS:HB2	1:C:237:PRO:HD2	1.97	0.46
1:C:542:VAL:HG21	1:C:551:TYR:OH	2.16	0.46
1:C:79:VAL:HG23	1:C:90:ARG:O	2.16	0.46
1:D:463:ALA:HB2	1:D:498:THR:O	2.15	0.46
1:D:464:LEU:CG	1:D:465:GLY:N	2.79	0.46
1:D:516:ILE:HD13	1:D:524:TYR:HB3	1.98	0.46
1:D:572:THR:HG22	1:D:576:LYS:O	2.16	0.46
1:A:264:GLY:O	1:A:265:LEU:HD23	2.16	0.46
1:B:208:LEU:O	1:B:209:TYR:C	2.56	0.46
1:B:209:TYR:O	1:B:210:LEU:C	2.59	0.46
1:B:247:SER:O	1:B:249:LEU:HD13	2.16	0.46
1:C:233:LEU:HD21	1:C:253:ARG:NH2	2.31	0.46
1:D:194:ILE:HA	1:D:603:GLY:O	2.15	0.46
1:D:223:THR:O	1:D:224:SER:HB2	2.15	0.46
1:D:72:ASN:N	1:D:72:ASN:ND2	2.59	0.46
1:D:107:ILE:HD11	1:D:118:TYR:CE2	2.51	0.46
1:A:395:GLU:OE1	1:A:395:GLU:O	2.34	0.45
1:A:98:PHE:CG	1:A:99:TYR:N	2.83	0.45
1:B:545:PRO:O	1:B:546:SER:C	2.59	0.45
1:C:208:LEU:O	1:C:212:ARG:HG2	2.16	0.45
1:C:434:LEU:HD13	1:C:495:HIS:O	2.16	0.45
1:C:481:TYR:CD2	1:C:482:ARG:HG2	2.51	0.45
1:C:123:GLU:HG2	1:C:128:VAL:HG23	1.98	0.45
1:D:63:VAL:HG12	1:D:64:VAL:N	2.30	0.45
1:A:282:ASN:OD1	1:A:284:LEU:HB2	2.16	0.45
1:A:393:LEU:HD12	1:A:393:LEU:O	2.16	0.45
1:A:585:LEU:N	1:A:585:LEU:CD2	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLU:CG	1:A:590:SER:N	2.78	0.45
1:A:589:GLU:O	1:A:591:GLY:N	2.46	0.45
1:C:236:LYS:NZ	1:C:277:GLU:OE1	2.42	0.45
1:D:593:HIS:HB2	2:D:901:NAG:O7	2.16	0.45
1:A:224:SER:C	1:A:226:GLY:H	2.24	0.45
1:A:366:ALA:O	1:A:441:MET:HB3	2.16	0.45
1:A:395:GLU:H	1:A:395:GLU:HG3	1.56	0.45
1:B:215:ASN:HB3	1:B:235:GLU:HB2	1.99	0.45
1:B:294:LEU:O	1:B:326:VAL:HG12	2.17	0.45
1:B:522:LEU:O	1:B:545:PRO:HD2	2.17	0.45
1:C:219:ILE:HG22	1:C:219:ILE:O	2.16	0.45
1:D:304:ASP:HB2	1:D:351:LEU:O	2.17	0.45
1:D:347:ASP:CG	1:D:406:ARG:HH22	2.24	0.45
1:D:461:ASN:H	1:D:461:ASN:ND2	2.15	0.45
1:A:473:ILE:HG22	1:A:474:PRO:CD	2.46	0.45
1:A:573:TRP:O	1:A:574:ASP:CB	2.62	0.45
1:B:406:ARG:O	1:B:408:PRO:HD3	2.17	0.45
1:B:35:ILE:HA	1:C:334:GLN:O	2.16	0.45
1:C:533:ARG:HB3	1:C:61:HIS:CD2	2.51	0.45
1:D:379:GLU:HG3	1:D:380:THR:H	1.82	0.45
1:D:574:ASP:C	1:D:576:LYS:H	2.25	0.45
1:A:301:HIS:HB2	1:A:319:PHE:CE2	2.51	0.45
1:B:265:LEU:HD11	1:D:209:TYR:CE2	2.52	0.45
1:B:276:LEU:HD23	1:B:277:GLU:N	2.31	0.45
1:B:36:VAL:HG11	1:C:333:MET:SD	2.57	0.45
1:C:236:LYS:HD3	1:C:252:TYR:CD2	2.52	0.45
1:C:510:LEU:HD12	1:C:563:PRO:HB2	1.99	0.45
1:D:200:ASN:HD22	1:D:200:ASN:N	2.10	0.45
1:D:206:LEU:HG	1:D:232:TYR:CZ	2.52	0.45
1:D:306:ILE:HD12	1:D:306:ILE:H	1.81	0.45
1:C:315:LYS:O	1:C:315:LYS:HG3	2.16	0.45
1:C:467:ILE:HD12	1:C:483:PHE:HE2	1.82	0.45
1:C:570:CYS:HA	1:C:578:TRP:O	2.16	0.45
1:C:119:PHE:HA	1:C:131:PHE:O	2.15	0.45
1:C:123:GLU:HA	1:C:128:VAL:HG23	1.99	0.45
1:D:472:TRP:C	1:D:474:PRO:HD2	2.42	0.45
1:D:499:TYR:CE2	1:D:501:PRO:HD3	2.51	0.45
1:D:65:THR:OG1	1:D:66:MET:N	2.49	0.45
1:A:466:VAL:HG12	1:A:468:ASN:ND2	2.32	0.45
1:A:559:ILE:H	1:A:559:ILE:CD1	2.28	0.45
1:A:32:CYS:SG	1:A:133:LEU:N	2.90	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LYS:NZ	1:B:277:GLU:OE2	2.41	0.45
1:B:274:ASN:ND2	1:B:324:LEU:HG	2.32	0.45
1:B:454:LEU:C	1:B:454:LEU:HD23	2.41	0.45
1:C:536:HIS:CE1	1:C:560:LYS:HB3	2.51	0.45
1:C:540:TYR:O	1:C:552:PHE:HA	2.17	0.45
1:D:526:LEU:HD12	1:D:526:LEU:O	2.15	0.45
1:D:99:TYR:O	1:D:103:LEU:N	2.50	0.45
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.31	0.45
1:B:473:ILE:CB	1:B:474:PRO:HD3	2.34	0.45
1:C:253:ARG:HD3	1:C:287:CYS:SG	2.57	0.45
1:D:369:THR:OG1	1:D:411:GLY:HA3	2.17	0.45
1:B:529:TYR:CE1	1:B:563:PRO:HD3	2.51	0.45
1:C:558:PRO:HD2	1:C:596:HIS:NE2	2.32	0.45
1:A:505:ASP:OD2	1:A:77:LYS:HD3	2.18	0.44
1:B:194:ILE:N	1:B:194:ILE:HD12	2.32	0.44
1:B:252:TYR:N	1:B:252:TYR:CD2	2.85	0.44
1:B:362:GLN:HB3	1:B:364:LYS:HE2	1.99	0.44
1:C:211:GLY:C	1:C:213:GLY:H	2.24	0.44
1:C:223:THR:O	1:C:224:SER:HB2	2.17	0.44
1:C:248:GLN:N	1:C:248:GLN:CD	2.75	0.44
1:C:564:ILE:HD11	1:C:584:VAL:CG1	2.47	0.44
1:A:323:LYS:C	1:A:324:LEU:HD12	2.42	0.44
1:A:444:TYR:CD2	1:A:516:ILE:HG12	2.52	0.44
1:A:36:VAL:O	1:A:37:GLN:HG2	2.18	0.44
1:A:52:ILE:HB	1:D:302:GLY:HA3	2.00	0.44
1:A:93:LYS:CD	1:A:94:ASP:N	2.76	0.44
1:B:558:PRO:HG2	1:B:559:ILE:N	2.32	0.44
1:B:48:THR:O	1:B:50:GLU:N	2.48	0.44
1:C:367:VAL:O	1:C:369:THR:HG23	2.17	0.44
1:C:386:CYS:O	1:C:391:GLN:HA	2.16	0.44
1:D:254:VAL:HG12	1:D:255:PHE:N	2.32	0.44
1:D:498:THR:CG2	1:D:499:TYR:N	2.80	0.44
1:A:308:ILE:HG23	1:A:309:PRO:HD2	1.98	0.44
1:A:461:ASN:HD22	1:A:461:ASN:C	2.24	0.44
1:B:311:GLN:CD	1:B:311:GLN:H	2.26	0.44
1:B:548:SER:C	1:B:550:SER:N	2.73	0.44
1:C:368:PRO:HD3	1:C:441:MET:HE3	2.00	0.44
1:C:406:ARG:HG3	1:C:406:ARG:HH11	1.82	0.44
1:C:565:GLU:HB3	1:C:584:VAL:CG2	2.47	0.44
1:A:310:TYR:O	1:A:312:GLY:N	2.47	0.44
1:A:93:LYS:CG	1:A:94:ASP:N	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:O	1:A:103:LEU:HD23	2.17	0.44
1:B:386:CYS:SG	1:B:386:CYS:O	2.74	0.44
1:C:205:LEU:HB2	1:C:272:MET:CE	2.43	0.44
1:C:276:LEU:HD12	1:C:276:LEU:HA	1.85	0.44
1:C:306:ILE:HG12	1:C:319:PHE:HE1	1.83	0.44
1:D:453:TRP:CH2	1:D:522:LEU:HD13	2.53	0.44
1:D:572:THR:HA	1:D:577:LEU:HA	1.98	0.44
1:D:96:TYR:CD2	1:D:107:ILE:HG12	2.53	0.44
1:A:325:GLY:C	1:A:327:TRP:N	2.73	0.44
1:A:384:GLN:CG	1:A:490:ALA:HB2	2.46	0.44
1:B:418:SER:O	1:B:419:LEU:HB2	2.18	0.44
1:B:458:PRO:HB3	1:B:464:LEU:HA	1.98	0.44
1:D:545:PRO:O	1:D:547:ARG:N	2.51	0.44
1:D:103:LEU:HD22	1:D:120:MET:SD	2.57	0.44
1:D:135:LEU:HD12	1:D:136:LYS:N	2.31	0.44
1:A:455:THR:HG22	1:A:516:ILE:HD11	1.98	0.44
1:A:472:TRP:HE3	1:A:473:ILE:HG12	1.81	0.44
1:B:337:VAL:HA	1:B:338:PRO:HD3	1.88	0.44
1:B:533:ARG:HG3	1:B:533:ARG:NH1	2.31	0.44
1:C:503:GLU:OE1	1:C:76:ASN:HB3	2.18	0.44
1:C:30:MET:C	1:C:32:CYS:H	2.24	0.44
1:C:48:THR:CG2	1:C:103:LEU:HB2	2.47	0.44
1:D:136:LYS:HG2	1:D:137:LEU:N	2.33	0.44
1:A:399:TRP:HZ3	1:A:435:ILE:HG22	1.81	0.44
1:B:327:TRP:O	1:B:328:LYS:C	2.61	0.44
1:D:260:ILE:HG12	1:D:270:PHE:CE1	2.52	0.44
1:D:288:MET:O	1:D:298:ALA:HA	2.18	0.44
1:D:400:ALA:HB3	1:D:401:PRO:CD	2.48	0.44
1:D:450:ASN:ND2	1:D:473:ILE:CG2	2.81	0.44
1:D:585:LEU:HD12	1:D:594:ILE:HG22	1.99	0.44
1:D:596:HIS:ND1	1:D:596:HIS:C	2.74	0.44
1:A:569:GLU:HG3	1:A:580:ARG:HG2	2.00	0.44
1:A:38:GLN:HB3	1:A:41:SER:HB3	2.00	0.44
1:C:206:LEU:HD22	1:C:210:LEU:CD1	2.48	0.44
1:C:288:MET:HB2	1:C:365:TRP:CD1	2.52	0.44
1:C:569:GLU:O	1:C:579:CYS:HA	2.18	0.44
1:C:91:TYR:HB3	1:C:93:LYS:CG	2.48	0.44
1:C:131:PHE:N	1:C:131:PHE:CD1	2.85	0.44
1:D:206:LEU:HD23	1:D:210:LEU:HG	1.99	0.44
1:B:229:GLY:H	1:B:291:LEU:HD11	1.81	0.44
1:B:299:LEU:HD11	1:B:425:ILE:CD1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:O	1:C:74:VAL:HG12	2.17	0.44
1:D:303:GLU:CG	1:D:304:ASP:H	2.29	0.44
1:D:375:LYS:CA	1:D:379:GLU:HB3	2.47	0.44
1:D:574:ASP:O	1:D:576:LYS:N	2.51	0.44
1:D:46:PRO:O	1:D:48:THR:N	2.51	0.44
1:C:416:ASP:OD1	1:C:416:ASP:C	2.60	0.43
1:D:585:LEU:HD12	1:D:585:LEU:O	2.18	0.43
1:D:94:ASP:HB3	1:D:95:ARG:H	1.41	0.43
1:A:378:MET:HA	1:A:378:MET:CE	2.43	0.43
1:A:570:CYS:HA	1:A:578:TRP:O	2.19	0.43
1:A:587:ASP:CG	1:A:588:SER:N	2.77	0.43
1:C:390:ILE:HG22	1:C:390:ILE:O	2.18	0.43
1:C:444:TYR:CZ	1:C:515:VAL:HA	2.54	0.43
1:C:459:MET:SD	1:C:459:MET:C	3.01	0.43
1:C:499:TYR:CE2	1:C:501:PRO:HB3	2.53	0.43
1:D:309:PRO:HG3	1:D:316:GLY:CA	2.44	0.43
1:A:580:ARG:HA	1:A:599:MET:HA	2.00	0.43
1:A:46:PRO:O	1:A:46:PRO:HG2	2.18	0.43
1:B:196:GLY:HA3	1:B:553:TYR:CZ	2.54	0.43
1:B:352:SER:OG	1:B:440:GLY:HA2	2.18	0.43
1:C:345:VAL:HG11	1:C:373:ASP:OD1	2.18	0.43
1:C:505:ASP:OD2	1:C:77:LYS:HE2	2.19	0.43
1:C:77:LYS:HG2	1:C:92:LEU:HD13	2.00	0.43
1:D:358:ILE:HA	1:D:362:GLN:O	2.18	0.43
1:D:405:ASN:N	1:D:405:ASN:HD22	2.15	0.43
1:D:538:VAL:HG23	1:D:557:LEU:HD11	2.00	0.43
1:A:312:GLY:O	1:A:314:GLY:N	2.44	0.43
1:A:507:ASP:CG	1:A:532:SER:HA	2.44	0.43
1:C:392:ALA:O	1:C:394:CYS:N	2.43	0.43
1:C:490:ALA:HB3	1:C:494:CYS:HB3	2.00	0.43
1:D:232:TYR:CD1	1:D:232:TYR:N	2.86	0.43
1:D:399:TRP:CD1	1:D:400:ALA:H	2.35	0.43
1:A:206:LEU:HD13	1:A:232:TYR:CD1	2.53	0.43
1:B:551:TYR:CD1	1:B:551:TYR:N	2.87	0.43
1:B:93:LYS:HD3	1:B:96:TYR:N	2.33	0.43
1:C:70:LEU:HD12	1:C:117:TRP:CE2	2.53	0.43
1:D:451:VAL:CG1	1:D:469:THR:HB	2.48	0.43
1:D:514:LEU:HD13	1:D:526:LEU:CD2	2.48	0.43
1:A:441:MET:HE2	1:A:456:ILE:HD11	2.00	0.43
1:C:514:LEU:HG	1:C:526:LEU:HD23	2.00	0.43
1:D:346:ILE:HG23	1:D:369:THR:CG2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:ILE:CD1	1:D:524:TYR:HB3	2.48	0.43
1:A:296:LEU:HD12	1:A:297:ALA:N	2.34	0.43
1:A:46:PRO:HA	1:A:104:SER:HA	2.00	0.43
1:B:400:ALA:CB	1:B:401:PRO:HD3	2.42	0.43
1:B:475:ARG:C	1:B:475:ARG:HD2	2.44	0.43
1:B:481:TYR:O	1:B:482:ARG:CG	2.64	0.43
1:B:81:LEU:C	1:B:81:LEU:HD12	2.43	0.43
1:C:39:LEU:HG	1:C:138:TYR:O	2.19	0.43
1:C:117:TRP:NE1	1:C:134:HIS:HB2	2.34	0.43
1:D:412:VAL:N	1:D:428:ALA:O	2.36	0.43
1:D:85:GLU:CD	1:D:85:GLU:H	2.27	0.43
1:D:139:GLU:OE1	1:D:139:GLU:HA	2.19	0.43
1:A:507:ASP:CG	1:A:90:ARG:HH12	2.27	0.43
1:A:556:ARG:HH22	1:A:125:ASN:HB2	1.83	0.43
1:A:573:TRP:O	1:A:574:ASP:HB3	2.19	0.43
1:A:58:LYS:HG3	1:A:58:LYS:O	2.18	0.43
1:B:276:LEU:HD23	1:B:276:LEU:C	2.43	0.43
1:B:508:VAL:HG13	1:B:528:THR:HG23	2.00	0.43
1:C:462:LEU:HB2	1:C:463:ALA:H	1.69	0.43
1:C:593:HIS:HD2	2:C:901:NAG:H81	1.83	0.43
1:A:387:LYS:HA	1:A:387:LYS:CE	2.49	0.43
1:A:50:GLU:HG2	1:A:52:ILE:HG23	2.00	0.43
1:A:69:SER:OG	1:A:70:LEU:N	2.51	0.43
1:B:66:MET:HG3	1:B:118:TYR:CZ	2.54	0.43
1:C:319:PHE:HB2	1:C:425:ILE:HD12	2.01	0.43
1:C:467:ILE:HB	1:C:482:ARG:HB2	2.00	0.43
1:C:508:VAL:HG23	1:C:528:THR:OG1	2.17	0.43
1:C:580:ARG:NH1	1:C:597:SER:OG	2.52	0.43
1:C:39:LEU:O	1:C:41:SER:N	2.51	0.43
1:D:74:VAL:O	1:D:74:VAL:HG12	2.19	0.43
1:D:78:ILE:C	1:D:92:LEU:HD21	2.44	0.43
1:B:533:ARG:NH2	1:B:554:PRO:HB3	2.34	0.43
1:C:91:TYR:C	1:C:93:LYS:N	2.73	0.43
1:D:346:ILE:HG23	1:D:369:THR:HG22	2.01	0.43
1:D:346:ILE:HA	1:D:371:ARG:HG2	2.01	0.43
1:D:473:ILE:N	1:D:474:PRO:HD2	2.34	0.43
1:D:482:ARG:HD2	1:D:72:ASN:ND2	2.34	0.43
1:A:473:ILE:HD13	1:A:473:ILE:HA	1.88	0.42
1:A:551:TYR:HD2	1:A:552:PHE:N	2.16	0.42
1:A:70:LEU:HA	1:A:73:SER:HB2	2.01	0.42
1:B:343:ASP:OD2	1:B:345:VAL:HB	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ALA:C	1:B:387:LYS:H	2.28	0.42
1:B:443:LEU:HD22	1:B:452:TYR:HB3	2.01	0.42
1:B:512:SER:HG	1:B:527:ALA:H	1.66	0.42
1:B:538:VAL:HG23	1:B:557:LEU:HD11	2.01	0.42
1:D:375:LYS:NZ	1:D:405:ASN:HB3	2.33	0.42
1:D:388:GLY:O	1:D:391:GLN:HB2	2.18	0.42
1:D:566:LEU:O	1:D:566:LEU:HG	2.19	0.42
1:B:340:SER:HB2	1:B:424:LYS:HD3	2.01	0.42
1:B:51:ARG:C	1:B:53:ASN:N	2.75	0.42
1:C:286:ASN:O	1:C:300:CYS:HA	2.18	0.42
1:C:290:ALA:HB2	1:C:365:TRP:CZ2	2.54	0.42
1:D:461:ASN:O	1:D:504:VAL:CG2	2.67	0.42
1:A:427:ILE:HG12	1:A:428:ALA:N	2.35	0.42
1:A:440:GLY:O	1:A:457:PRO:HD2	2.19	0.42
1:A:539:VAL:HA	1:A:553:TYR:O	2.18	0.42
1:B:395:GLU:O	1:B:396:ASN:HB2	2.19	0.42
1:B:418:SER:O	1:B:419:LEU:CB	2.67	0.42
1:B:558:PRO:HG2	1:B:559:ILE:H	1.84	0.42
1:B:559:ILE:H	1:B:559:ILE:CD1	2.32	0.42
1:D:61:HIS:HE1	1:D:63:VAL:CG2	2.32	0.42
1:B:265:LEU:HD11	1:D:209:TYR:HE2	1.83	0.42
1:B:400:ALA:CB	1:B:401:PRO:CD	2.95	0.42
1:B:470:LEU:HD11	1:B:476:PHE:CE1	2.55	0.42
1:C:399:TRP:O	1:C:400:ALA:C	2.62	0.42
1:A:406:ARG:O	1:A:408:PRO:HD3	2.20	0.42
1:A:38:GLN:O	1:A:39:LEU:C	2.63	0.42
1:B:233:LEU:HD23	1:B:253:ARG:HA	2.01	0.42
1:D:437:HIS:HB3	1:D:459:MET:CG	2.39	0.42
1:C:206:LEU:O	1:C:207:ASP:C	2.60	0.42
1:C:337:VAL:CG1	1:C:338:PRO:HD2	2.49	0.42
1:D:252:TYR:CE1	1:D:279:PRO:HB3	2.54	0.42
1:D:301:HIS:CE1	1:D:306:ILE:HG13	2.54	0.42
1:D:320:GLN:HB2	1:D:336:TRP:CZ3	2.53	0.42
1:D:461:ASN:C	1:D:462:LEU:HD23	2.45	0.42
1:A:208:LEU:O	1:A:209:TYR:C	2.62	0.42
1:A:388:GLY:O	1:A:389:LYS:C	2.62	0.42
1:B:371:ARG:HH11	1:B:429:SER:HB3	1.84	0.42
1:B:59:SER:O	1:B:61:HIS:N	2.53	0.42
1:C:229:GLY:HA2	1:C:256:GLU:O	2.20	0.42
1:C:464:LEU:HD22	1:C:498:THR:O	2.19	0.42
1:C:537:ALA:CB	1:C:556:ARG:HA	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LEU:HD13	1:D:251:MET:CE	2.50	0.42
1:D:326:VAL:HG13	1:D:327:TRP:H	1.84	0.42
1:D:385:ALA:O	1:D:390:ILE:HG12	2.20	0.42
1:D:111:THR:OG1	1:D:112:LYS:N	2.53	0.42
1:A:400:ALA:HB3	1:A:401:PRO:CD	2.50	0.42
1:B:464:LEU:CG	1:B:465:GLY:N	2.79	0.42
1:B:487:ILE:HG22	1:B:490:ALA:HB3	2.01	0.42
1:C:453:TRP:CB	1:C:516:ILE:HD12	2.50	0.42
1:D:262:ASN:HB2	1:D:573:TRP:HZ2	1.84	0.42
1:D:49:HIS:O	1:D:50:GLU:HG3	2.19	0.42
1:A:265:LEU:HD22	1:C:214:TYR:CZ	2.55	0.42
1:A:356:GLY:HA3	1:A:364:LYS:O	2.19	0.42
1:A:552:PHE:HE1	1:A:121:THR:OG1	2.00	0.42
1:B:229:GLY:HA3	1:B:291:LEU:HD21	2.02	0.42
1:C:473:ILE:HG22	1:C:474:PRO:CD	2.49	0.42
1:C:61:HIS:CE1	1:C:63:VAL:CG2	3.03	0.42
1:C:81:LEU:HD13	1:C:81:LEU:C	2.45	0.42
1:D:307:THR:HA	1:D:348:ARG:CG	2.50	0.42
1:D:340:SER:HB3	1:D:426:LYS:HA	2.01	0.42
1:D:559:ILE:CG1	1:D:560:LYS:H	2.33	0.42
1:A:38:GLN:CG	1:D:422:GLU:HB3	2.49	0.42
1:A:124:LYS:HB2	1:A:127:SER:HB2	2.02	0.42
1:B:374:ASP:CG	1:B:375:LYS:H	2.27	0.42
1:B:548:SER:O	1:B:550:SER:N	2.53	0.42
1:B:32:CYS:O	1:B:33:PRO:C	2.60	0.42
1:C:293:GLU:OE2	1:C:358:ILE:HG22	2.19	0.42
1:C:392:ALA:C	1:C:394:CYS:N	2.75	0.42
1:D:445:LYS:HA	1:D:452:TYR:CD2	2.55	0.42
1:D:586:ALA:HB2	1:D:593:HIS:CE1	2.55	0.42
1:D:37:GLN:NE2	1:D:43:VAL:CA	2.70	0.42
1:A:365:TRP:O	1:A:412:VAL:HA	2.19	0.41
1:A:538:VAL:HB	1:A:555:PHE:HB3	2.02	0.41
1:B:470:LEU:HD13	1:B:478:VAL:CG2	2.50	0.41
1:C:418:SER:C	1:C:420:THR:N	2.77	0.41
1:C:97:ARG:HB3	1:C:106:ALA:HB3	2.02	0.41
1:D:384:GLN:NE2	1:D:489:GLU:HB2	2.35	0.41
1:D:516:ILE:HD13	1:D:524:TYR:CB	2.50	0.41
1:D:37:GLN:O	1:D:38:GLN:C	2.63	0.41
1:D:81:LEU:CD1	1:D:89:PRO:HG2	2.50	0.41
1:A:205:LEU:HG	1:A:209:TYR:CE1	2.54	0.41
1:B:379:GLU:HA	1:B:407:ILE:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LEU:O	1:C:208:LEU:HB3	2.20	0.41
1:C:39:LEU:O	1:C:110:SER:OG	2.35	0.41
1:C:95:ARG:NH1	1:C:95:ARG:HG2	2.35	0.41
1:A:383:GLN:HA	1:A:386:CYS:HB2	2.02	0.41
1:A:533:ARG:NH1	1:A:554:PRO:CB	2.82	0.41
1:A:47:LEU:N	1:A:47:LEU:HD13	2.34	0.41
1:B:62:ILE:N	1:B:62:ILE:CD1	2.82	0.41
1:C:293:GLU:OE1	1:C:360:ASP:N	2.48	0.41
1:A:327:TRP:CZ3	1:C:328:LYS:HD3	2.56	0.41
1:A:379:GLU:OE1	1:A:379:GLU:HA	2.20	0.41
1:B:524:TYR:CD2	1:B:524:TYR:N	2.88	0.41
1:B:546:SER:OG	1:B:547:ARG:N	2.53	0.41
1:C:536:HIS:CD2	1:C:560:LYS:HG2	2.56	0.41
1:D:357:VAL:HG22	1:D:358:ILE:N	2.35	0.41
1:C:233:LEU:HD21	1:C:253:ARG:CZ	2.50	0.41
1:D:298:ALA:HB3	1:D:322:VAL:HB	2.01	0.41
1:D:125:ASN:OD1	1:D:126:ILE:N	2.46	0.41
1:A:198:PHE:N	1:A:198:PHE:CD2	2.89	0.41
1:A:418:SER:O	1:A:419:LEU:HB2	2.21	0.41
1:B:348:ARG:HD3	1:B:350:TYR:CZ	2.56	0.41
1:B:139:GLU:O	1:B:140:GLN:CB	2.63	0.41
1:C:389:LYS:HE3	1:C:500:LEU:N	2.30	0.41
1:C:30:MET:O	1:C:32:CYS:N	2.53	0.41
1:D:248:GLN:HG2	1:D:249:LEU:N	2.36	0.41
1:A:251:MET:HE3	1:A:283:ASP:HB3	2.03	0.41
1:A:455:THR:HG21	1:A:516:ILE:HD11	2.03	0.41
1:B:385:ALA:C	1:B:387:LYS:N	2.79	0.41
1:B:433:PRO:O	1:B:434:LEU:C	2.64	0.41
1:B:466:VAL:CG1	1:B:468:ASN:HD21	2.34	0.41
1:C:406:ARG:HG3	1:C:406:ARG:NH1	2.35	0.41
1:C:420:THR:C	1:C:421:VAL:HG13	2.45	0.41
1:D:542:VAL:HB	1:D:551:TYR:CE1	2.56	0.41
1:A:229:GLY:N	1:A:291:LEU:HD11	2.35	0.41
1:A:255:PHE:HB2	1:A:276:LEU:HB3	2.01	0.41
1:B:400:ALA:O	1:B:401:PRO:C	2.63	0.41
1:B:486:PRO:HA	1:B:495:HIS:ND1	2.36	0.41
1:C:261:ARG:NH1	1:C:271:HIS:ND1	2.68	0.41
1:C:488:LYS:O	1:C:489:GLU:C	2.64	0.41
1:C:575:GLN:HE21	1:C:575:GLN:HB2	1.70	0.41
1:D:348:ARG:HG2	1:D:348:ARG:HH11	1.86	0.41
1:D:386:CYS:HA	1:D:390:ILE:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:ILE:HG12	1:D:560:LYS:O	2.21	0.41
1:A:227:MET:HE1	1:A:294:LEU:N	2.33	0.41
1:A:308:ILE:HA	1:A:309:PRO:HD3	1.94	0.41
1:A:378:MET:HB3	1:A:407:ILE:CD1	2.51	0.41
1:A:569:GLU:O	1:A:579:CYS:HA	2.20	0.41
1:A:569:GLU:CG	1:A:580:ARG:HG2	2.50	0.41
1:A:103:LEU:HD13	1:A:120:MET:SD	2.61	0.41
1:B:203:LEU:HB2	1:B:271:HIS:HA	2.03	0.41
1:B:352:SER:H	1:B:354:HIS:CD2	2.38	0.41
1:B:392:ALA:HA	1:B:395:GLU:OE1	2.21	0.41
1:B:488:LYS:O	1:B:489:GLU:C	2.64	0.41
1:B:500:LEU:HD22	1:B:502:ALA:HB3	2.02	0.41
1:B:36:VAL:O	1:B:37:GLN:CG	2.69	0.41
1:C:260:ILE:HG12	1:C:270:PHE:CE1	2.56	0.41
1:C:376:LEU:HD23	1:C:376:LEU:C	2.45	0.41
1:C:572:THR:HA	1:C:577:LEU:HA	2.03	0.41
1:C:38:GLN:O	1:C:39:LEU:C	2.64	0.41
1:C:48:THR:OG1	1:C:49:HIS:N	2.54	0.41
1:C:61:HIS:HE1	1:C:63:VAL:CG2	2.34	0.41
1:C:88:PRO:HA	1:C:89:PRO:HD2	1.81	0.41
1:C:99:TYR:C	1:C:101:GLU:HG2	2.46	0.41
1:D:454:LEU:HD23	1:D:454:LEU:C	2.45	0.41
1:D:520:GLN:CG	1:D:521:ASP:N	2.83	0.41
1:D:542:VAL:HG21	1:D:551:TYR:OH	2.21	0.41
1:D:30:MET:O	1:D:30:MET:HG3	2.21	0.41
1:D:99:TYR:HB2	1:D:104:SER:OG	2.21	0.41
1:B:103:LEU:CD1	1:B:120:MET:HE1	2.47	0.41
1:B:129:GLN:HG2	1:B:131:PHE:CE1	2.55	0.41
1:C:308:ILE:CD1	1:C:349:LEU:HD12	2.47	0.41
1:C:407:ILE:N	1:C:407:ILE:HD12	2.35	0.41
1:C:37:GLN:CG	1:C:43:VAL:HG12	2.47	0.41
1:D:530:ASP:OD1	1:D:532:SER:HB3	2.21	0.41
1:A:197:GLN:NE2	1:A:266:GLY:O	2.51	0.40
1:A:387:LYS:HA	1:A:387:LYS:HE2	2.03	0.40
1:A:580:ARG:HA	1:A:598:GLY:O	2.21	0.40
1:A:72:ASN:O	1:A:74:VAL:N	2.55	0.40
1:B:337:VAL:O	1:B:337:VAL:HG23	2.19	0.40
1:B:540:TYR:CE1	1:B:568:VAL:HG21	2.54	0.40
1:B:562:VAL:HG23	1:B:586:ALA:O	2.21	0.40
1:B:570:CYS:HA	1:B:578:TRP:O	2.21	0.40
1:B:100:LEU:HD13	1:B:100:LEU:C	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:ILE:O	1:C:516:ILE:HG22	2.20	0.40
1:D:231:THR:OG1	1:D:253:ARG:NH1	2.54	0.40
1:D:418:SER:C	1:D:420:THR:N	2.77	0.40
1:D:472:TRP:CG	1:D:473:ILE:H	2.39	0.40
1:A:107:ILE:HD11	1:A:118:TYR:CE2	2.57	0.40
1:B:343:ASP:C	1:B:345:VAL:H	2.29	0.40
1:B:392:ALA:HA	1:B:395:GLU:HG2	2.03	0.40
1:B:65:THR:OG1	1:B:119:PHE:HB2	2.21	0.40
1:B:93:LYS:HB2	1:B:96:TYR:H	1.86	0.40
1:C:473:ILE:N	1:C:474:PRO:CD	2.84	0.40
1:C:526:LEU:C	1:C:526:LEU:CD1	2.94	0.40
1:A:310:TYR:N	1:A:310:TYR:CD2	2.89	0.40
1:B:395:GLU:O	1:B:395:GLU:HG3	2.21	0.40
1:B:579:CYS:O	1:B:599:MET:HA	2.20	0.40
1:C:488:LYS:O	1:C:489:GLU:HG2	2.22	0.40
1:C:91:TYR:HB3	1:C:93:LYS:CB	2.51	0.40
1:C:125:ASN:CG	1:C:126:ILE:H	2.29	0.40
1:D:474:PRO:O	1:D:475:ARG:HB3	2.21	0.40
1:D:562:VAL:HA	1:D:563:PRO:HD2	1.92	0.40
1:A:454:LEU:HD23	1:A:454:LEU:C	2.46	0.40
1:B:358:ILE:HA	1:B:362:GLN:O	2.21	0.40
1:C:508:VAL:HG13	1:C:508:VAL:O	2.20	0.40
1:D:230:GLY:HA2	1:D:289:VAL:HG11	2.02	0.40
1:D:307:THR:C	1:D:308:ILE:HD12	2.46	0.40
1:D:461:ASN:N	1:D:461:ASN:ND2	2.62	0.40
1:A:270:PHE:HE1	1:A:599:MET:HE1	1.82	0.40
1:A:500:LEU:C	1:A:502:ALA:N	2.78	0.40
1:B:236:LYS:O	1:B:249:LEU:O	2.39	0.40
1:B:294:LEU:HD12	1:B:326:VAL:HG11	2.03	0.40
1:B:308:ILE:N	1:B:308:ILE:CD1	2.85	0.40
1:C:236:LYS:O	1:C:249:LEU:HB3	2.21	0.40
1:C:412:VAL:CG2	1:C:476:PHE:HE1	2.34	0.40
1:C:493:ASP:HB2	1:C:495:HIS:NE2	2.36	0.40
1:C:535:GLU:OE2	1:C:556:ARG:HD3	2.22	0.40
1:C:65:THR:CG2	1:C:75:GLU:HB3	2.48	0.40
1:D:262:ASN:HB2	1:D:573:TRP:CZ2	2.57	0.40
1:D:333:MET:HE3	1:D:335:SER:HB2	2.03	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	509/559 (91%)	416 (82%)	62 (12%)	31 (6%)	1	7
1	B	520/559 (93%)	412 (79%)	86 (16%)	22 (4%)	2	13
1	C	504/559 (90%)	407 (81%)	67 (13%)	30 (6%)	1	8
1	D	492/559 (88%)	389 (79%)	70 (14%)	33 (7%)	1	6
All	All	2025/2236 (91%)	1624 (80%)	285 (14%)	116 (6%)	1	9

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	389	LYS
1	A	439	SER
1	A	490	ALA
1	A	494	CYS
1	A	502	ALA
1	A	548	SER
1	A	39	LEU
1	A	60	ILE
1	A	72	ASN
1	A	73	SER
1	A	85	GLU
1	A	93	LYS
1	A	94	ASP
1	B	476	PHE
1	B	512	SER
1	B	60	ILE
1	B	73	SER
1	B	74	VAL
1	B	93	LYS
1	C	236	LYS
1	C	237	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	449	ASN
1	C	549	PHE
1	C	31	ASN
1	C	39	LEU
1	C	93	LYS
1	D	309	PRO
1	D	347	ASP
1	D	376	LEU
1	D	460	LYS
1	D	497	PRO
1	D	547	ARG
1	D	38	GLN
1	D	86	ALA
1	D	94	ASP
1	A	438	GLY
1	A	475	ARG
1	A	574	ASP
1	A	590	SER
1	A	592	GLY
1	A	52	ILE
1	A	79	VAL
1	B	239	LEU
1	B	397	PRO
1	B	474	PRO
1	B	490	ALA
1	B	52	ILE
1	B	94	ASP
1	C	274	ASN
1	C	315	LYS
1	C	347	ASP
1	C	422	GLU
1	C	475	ARG
1	C	548	SER
1	C	50	GLU
1	D	374	ASP
1	D	437	HIS
1	D	465	GLY
1	D	475	ARG
1	D	522	LEU
1	D	546	SER
1	D	548	SER
1	D	575	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	39	LEU
1	D	47	LEU
1	D	59	SER
1	D	109	GLU
1	A	189	SER
1	A	451	VAL
1	A	53	ASN
1	A	133	LEU
1	B	222	MET
1	B	250	SER
1	B	489	GLU
1	C	393	LEU
1	C	40	GLY
1	C	101	GLU
1	D	390	ILE
1	D	92	LEU
1	A	390	ILE
1	B	238	ASN
1	B	481	TYR
1	C	460	LYS
1	C	125	ASN
1	C	133	LEU
1	D	224	SER
1	D	502	ALA
1	D	46	PRO
1	A	352	SER
1	A	75	GLU
1	A	84	SER
1	B	400	ALA
1	B	549	PHE
1	C	400	ALA
1	C	74	VAL
1	D	212	ARG
1	D	381	CYS
1	D	422	GLU
1	D	441	MET
1	D	68	LYS
1	A	473	ILE
1	B	390	ILE
1	C	462	LEU
1	C	46	PRO
1	C	83	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	94	ASP
1	D	492	GLY
1	C	316	GLY
1	C	500	LEU
1	D	43	VAL
1	B	401	PRO
1	C	35	ILE
1	A	492	GLY
1	C	60	ILE
1	B	226	GLY

5.3.2 Protein sidechains [i](#)

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	457/489 (94%)	403 (88%)	54 (12%)	5	20
1	B	468/489 (96%)	428 (92%)	40 (8%)	10	33
1	C	457/489 (94%)	403 (88%)	54 (12%)	5	20
1	D	449/489 (92%)	416 (93%)	33 (7%)	13	38
All	All	1831/1956 (94%)	1650 (90%)	181 (10%)	7	27

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	CYS
1	A	193	THR
1	A	195	ARG
1	A	221	THR
1	A	223	THR
1	A	261	ARG
1	A	273	THR
1	A	275	TYR
1	A	293	GLU
1	A	296	LEU
1	A	311	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	331	THR
1	A	341	THR
1	A	357	VAL
1	A	378	MET
1	A	379	GLU
1	A	381	CYS
1	A	384	GLN
1	A	387	LYS
1	A	395	GLU
1	A	398	GLU
1	A	413	LEU
1	A	449	ASN
1	A	461	ASN
1	A	471	GLU
1	A	472	TRP
1	A	473	ILE
1	A	479	SER
1	A	484	THR
1	A	488	LYS
1	A	489	GLU
1	A	494	CYS
1	A	514	LEU
1	A	518	PRO
1	A	520	GLN
1	A	521	ASP
1	A	549	PHE
1	A	559	ILE
1	A	564	ILE
1	A	580	ARG
1	A	604	VAL
1	A	38	GLN
1	A	45	LEU
1	A	47	LEU
1	A	48	THR
1	A	56	MET
1	A	70	LEU
1	A	80	SER
1	A	95	ARG
1	A	100	LEU
1	A	101	GLU
1	A	103	LEU
1	A	128	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	133	LEU
1	B	193	THR
1	B	217	SER
1	B	235	GLU
1	B	246	LEU
1	B	249	LEU
1	B	257	VAL
1	B	275	TYR
1	B	296	LEU
1	B	305	SER
1	B	310	TYR
1	B	342	ASP
1	B	357	VAL
1	B	413	LEU
1	B	419	LEU
1	B	449	ASN
1	B	459	MET
1	B	461	ASN
1	B	464	LEU
1	B	471	GLU
1	B	472	TRP
1	B	479	SER
1	B	484	THR
1	B	500	LEU
1	B	510	LEU
1	B	526	LEU
1	B	559	ILE
1	B	577	LEU
1	B	605	SER
1	B	34	LYS
1	B	38	GLN
1	B	45	LEU
1	B	48	THR
1	B	52	ILE
1	B	80	SER
1	B	92	LEU
1	B	93	LYS
1	B	101	GLU
1	B	105	LEU
1	B	133	LEU
1	B	137	LEU
1	C	192	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	200	ASN
1	C	206	LEU
1	C	221	THR
1	C	223	THR
1	C	227	MET
1	C	231	THR
1	C	234	VAL
1	C	248	GLN
1	C	249	LEU
1	C	282	ASN
1	C	296	LEU
1	C	299	LEU
1	C	320	GLN
1	C	349	LEU
1	C	351	LEU
1	C	355	ARG
1	C	357	VAL
1	C	376	LEU
1	C	391	GLN
1	C	414	SER
1	C	415	VAL
1	C	422	GLU
1	C	427	ILE
1	C	436	THR
1	C	449	ASN
1	C	451	VAL
1	C	455	THR
1	C	459	MET
1	C	461	ASN
1	C	464	LEU
1	C	473	ILE
1	C	479	SER
1	C	510	LEU
1	C	514	LEU
1	C	526	LEU
1	C	528	THR
1	C	533	ARG
1	C	547	ARG
1	C	568	VAL
1	C	572	THR
1	C	589	GLU
1	C	607	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	37	GLN
1	C	50	GLU
1	C	65	THR
1	C	70	LEU
1	C	72	ASN
1	C	93	LYS
1	C	95	ARG
1	C	101	GLU
1	C	102	HIS
1	C	132	CYS
1	C	136	LYS
1	D	193	THR
1	D	200	ASN
1	D	206	LEU
1	D	223	THR
1	D	299	LEU
1	D	306	ILE
1	D	315	LYS
1	D	331	THR
1	D	334	GLN
1	D	352	SER
1	D	360	ASP
1	D	377	ARG
1	D	427	ILE
1	D	437	HIS
1	D	455	THR
1	D	461	ASN
1	D	464	LEU
1	D	489	GLU
1	D	515	VAL
1	D	520	GLN
1	D	528	THR
1	D	549	PHE
1	D	557	LEU
1	D	572	THR
1	D	577	LEU
1	D	31	ASN
1	D	42	ASP
1	D	46	PRO
1	D	65	THR
1	D	72	ASN
1	D	93	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	95	ARG
1	D	112	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	286	ASN
1	A	311	GLN
1	A	391	GLN
1	A	448	HIS
1	A	449	ASN
1	A	461	ASN
1	A	468	ASN
1	A	37	GLN
1	A	57	ASN
1	A	72	ASN
1	A	76	ASN
1	A	129	GLN
1	B	262	ASN
1	B	278	GLN
1	B	320	GLN
1	B	334	GLN
1	B	361	ASN
1	B	362	GLN
1	B	383	GLN
1	B	384	GLN
1	B	449	ASN
1	B	461	ASN
1	B	468	ASN
1	B	575	GLN
1	B	596	HIS
1	B	37	GLN
1	B	61	HIS
1	B	125	ASN
1	B	140	GLN
1	C	262	ASN
1	C	286	ASN
1	C	383	GLN
1	C	384	GLN
1	C	461	ASN
1	C	468	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	523	GLN
1	C	567	GLN
1	C	575	GLN
1	C	581	HIS
1	C	593	HIS
1	C	37	GLN
1	C	61	HIS
1	C	72	ASN
1	C	129	GLN
1	D	200	ASN
1	D	248	GLN
1	D	278	GLN
1	D	286	ASN
1	D	320	GLN
1	D	383	GLN
1	D	405	ASN
1	D	461	ASN
1	D	468	ASN
1	D	520	GLN
1	D	523	GLN
1	D	536	HIS
1	D	575	GLN
1	D	593	HIS
1	D	37	GLN
1	D	49	HIS
1	D	61	HIS
1	D	72	ASN
1	D	76	ASN
1	D	102	HIS
1	D	134	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are 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	$\# Z > 2$
2	NAG	B	801	1	14,14,15	1.09	1 (7%)	17,19,21	0.81	0
2	NAG	C	901	1	14,14,15	0.75	0	17,19,21	0.82	0
2	NAG	D	901	1	14,14,15	0.97	1 (7%)	17,19,21	0.83	0
2	NAG	C	801	1	14,14,15	0.85	1 (7%)	17,19,21	0.59	0
2	NAG	B	901	1	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
2	NAG	A	901	1	14,14,15	0.88	1 (7%)	17,19,21	1.28	3 (17%)

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
2	NAG	B	801	1	-	4/6/23/26	0/1/1/1
2	NAG	C	901	1	-	2/6/23/26	0/1/1/1
2	NAG	D	901	1	-	5/6/23/26	0/1/1/1
2	NAG	C	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	901	1	-	4/6/23/26	0/1/1/1
2	NAG	A	901	1	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAG	C1-C2	3.43	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	NAG	C1-C2	2.40	1.55	1.52
2	A	901	NAG	C4-C5	2.14	1.57	1.53
2	C	801	NAG	C1-C2	2.10	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NAG	C3-C4-C5	2.95	115.58	110.23
2	A	901	NAG	C2-N2-C7	-2.62	119.39	122.90
2	B	901	NAG	C2-N2-C7	-2.45	119.62	122.90
2	A	901	NAG	O5-C1-C2	-2.19	107.91	111.29

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	NAG	C8-C7-N2-C2
2	A	901	NAG	O7-C7-N2-C2
2	B	801	NAG	C8-C7-N2-C2
2	B	801	NAG	O7-C7-N2-C2
2	C	801	NAG	C8-C7-N2-C2
2	C	801	NAG	O7-C7-N2-C2
2	C	901	NAG	C8-C7-N2-C2
2	C	901	NAG	O7-C7-N2-C2
2	D	901	NAG	C3-C2-N2-C7
2	D	901	NAG	C8-C7-N2-C2
2	D	901	NAG	O7-C7-N2-C2
2	C	801	NAG	O5-C5-C6-O6
2	D	901	NAG	O5-C5-C6-O6
2	D	901	NAG	C4-C5-C6-O6
2	B	901	NAG	C8-C7-N2-C2
2	B	901	NAG	O7-C7-N2-C2
2	C	801	NAG	C4-C5-C6-O6
2	B	901	NAG	O5-C5-C6-O6
2	B	901	NAG	C4-C5-C6-O6
2	A	901	NAG	C4-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6
2	A	901	NAG	O5-C5-C6-O6
2	B	801	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	NAG	1	0
2	D	901	NAG	1	0

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	515/559 (92%)	0.16	10 (1%) 66 45	33, 57, 97, 115	0
1	B	526/559 (94%)	0.25	13 (2%) 58 37	38, 66, 109, 122	0
1	C	514/559 (91%)	0.26	12 (2%) 61 40	39, 66, 101, 118	0
1	D	504/559 (90%)	0.36	15 (2%) 52 32	49, 75, 114, 130	0
All	All	2059/2236 (92%)	0.26	50 (2%) 59 39	33, 67, 108, 130	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	ILE	3.7
1	C	497	PRO	3.6
1	A	74	VAL	3.5
1	B	53	ASN	3.3
1	C	249	LEU	3.3
1	D	73	SER	3.2
1	B	503	GLU	3.1
1	B	393	LEU	3.0
1	B	59	SER	2.9
1	B	52	ILE	2.9
1	D	393	LEU	2.8
1	D	549	PHE	2.8
1	C	545	PRO	2.7
1	D	473	ILE	2.7
1	A	71	GLU	2.7
1	C	590	SER	2.7
1	D	559	ILE	2.6
1	A	503	GLU	2.6
1	A	438	GLY	2.6
1	B	474	PRO	2.5
1	B	550	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	575	GLN	2.5
1	C	313	SER	2.5
1	A	310	TYR	2.4
1	A	606	CYS	2.4
1	D	502	ALA	2.4
1	B	140	GLN	2.4
1	D	227	MET	2.4
1	D	472	TRP	2.4
1	C	393	LEU	2.3
1	C	317	VAL	2.2
1	B	587	ASP	2.2
1	B	54	THR	2.2
1	D	380	THR	2.2
1	A	549	PHE	2.2
1	B	74	VAL	2.2
1	C	449	ASN	2.2
1	D	449	ASN	2.2
1	B	249	LEU	2.1
1	D	83	PRO	2.1
1	C	549	PHE	2.1
1	D	376	LEU	2.1
1	A	237	PRO	2.1
1	D	313	SER	2.1
1	D	544	SER	2.1
1	C	189	SER	2.1
1	C	491	GLY	2.1
1	C	73	SER	2.0
1	A	311	GLN	2.0
1	B	252	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	NAG	C	801	14/15	0.48	0.18	90,94,98,98	0
2	NAG	D	901	14/15	0.50	0.17	95,98,103,105	0
2	NAG	B	801	14/15	0.55	0.15	89,91,93,93	0
2	NAG	C	901	14/15	0.57	0.15	94,97,99,99	0
2	NAG	B	901	14/15	0.65	0.15	100,102,104,104	0
2	NAG	A	901	14/15	0.71	0.13	88,90,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.