



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:06 AM UTC

PDB ID : 3L5N / pdb_00003l5n
Title : Staphylococcal Complement Inhibitor (SCIN) in complex with Human Complement Component C3b
Authors : Geisbrecht, B.V.; Garcia, B.L.
Deposited on : 2009-12-22
Resolution : 7.54 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

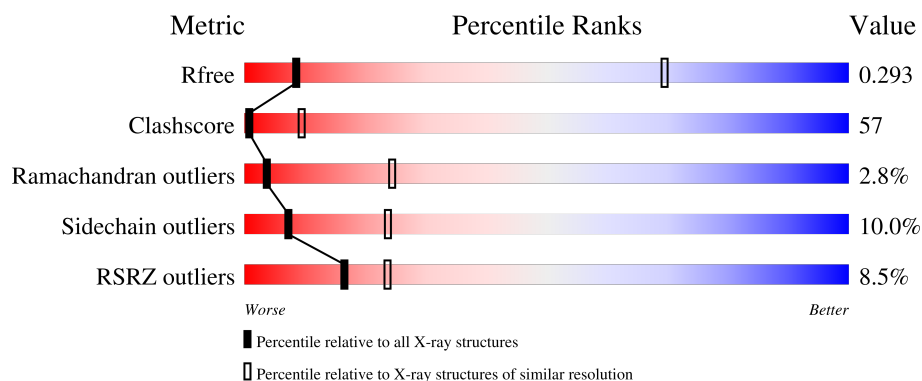
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.54 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	645	9% 33% 55% 10% ..
2	B	915	7% 42% 48% 7% .
3	M	88	3% 45% 44% 6% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12785 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 Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			4932	3143	833	941	15			

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	891	Total	C	N	O	S	1168	0	0
			7118	4512	1195	1373	38			

- Molecule 3 is a protein called Staphylococcal complement inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

There are 3 discrepancies between the modelled and reference sequences:

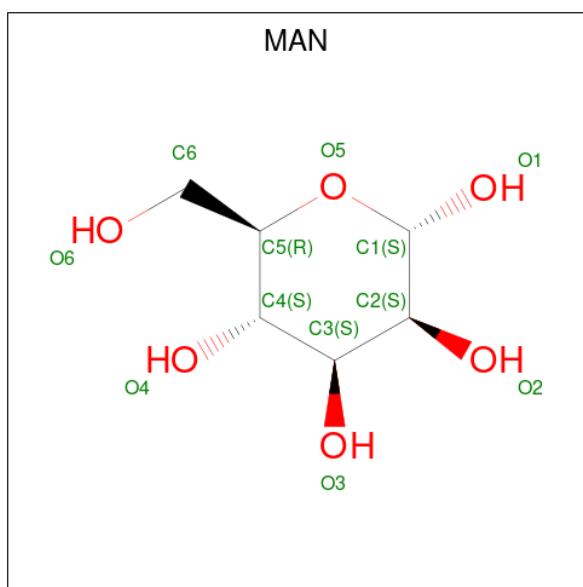
Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP Q931M7
M	-1	SER	-	expression tag	UNP Q931M7
M	0	THR	-	expression tag	UNP Q931M7

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).

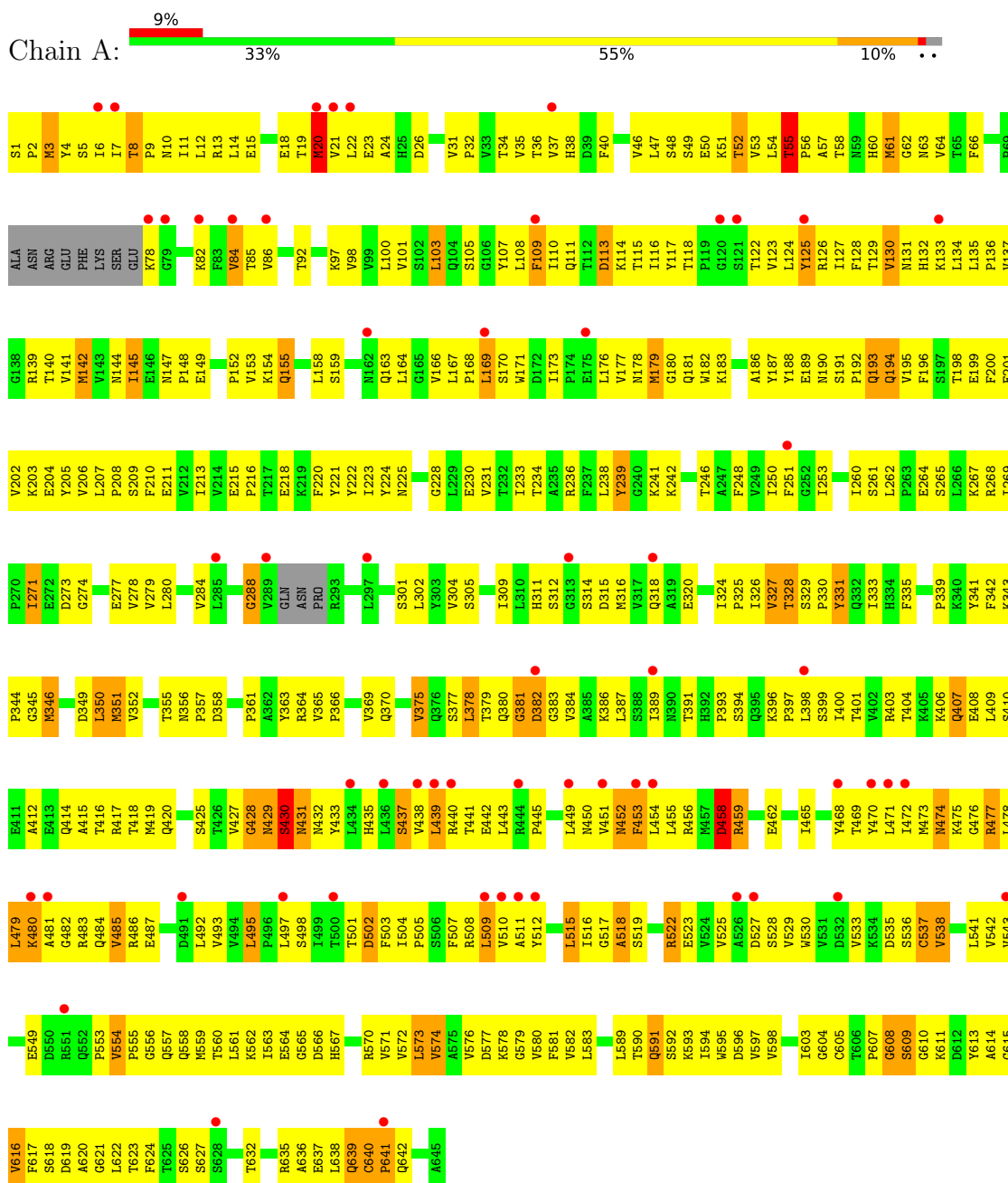


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

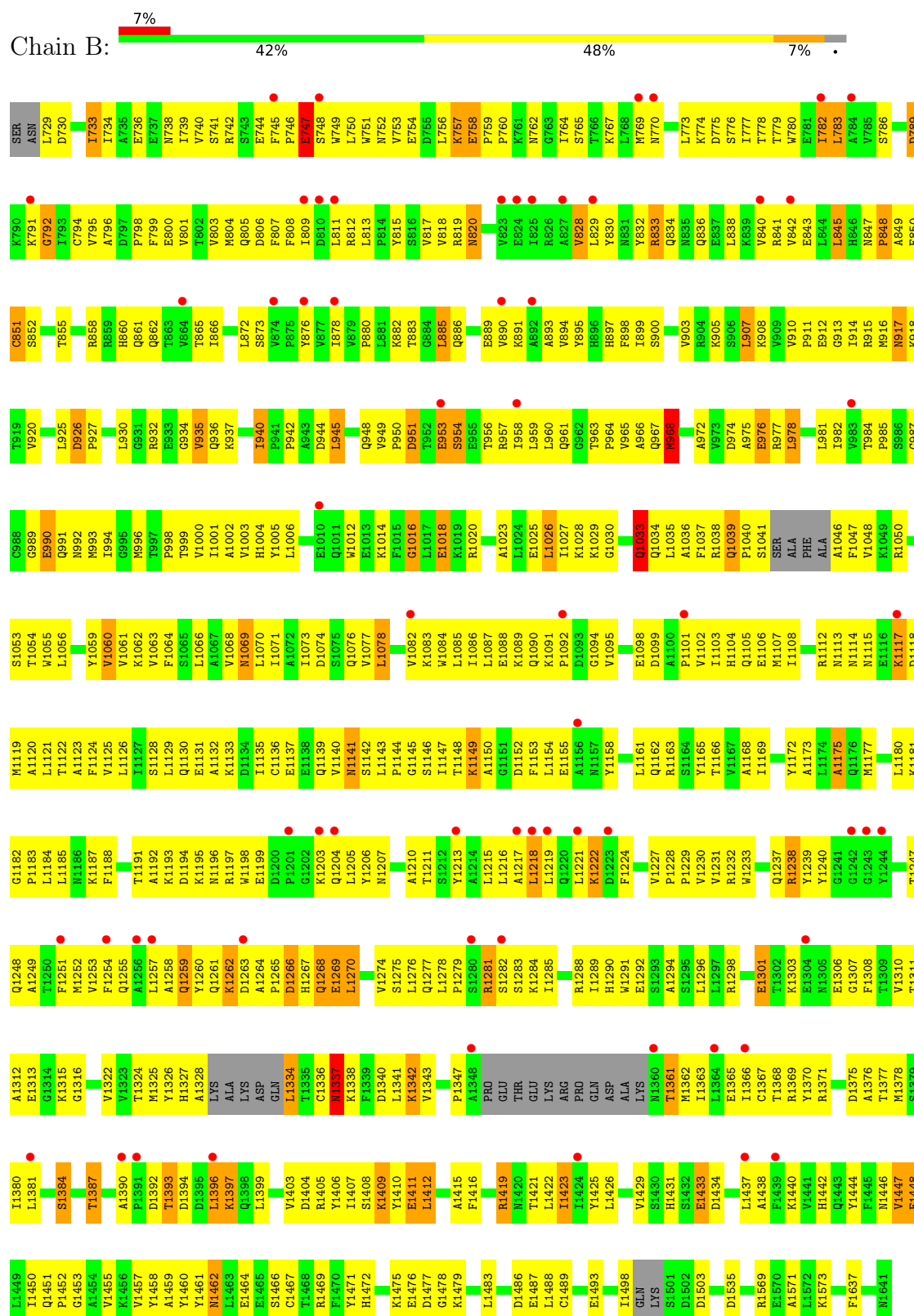
3 Residue-property plots

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.

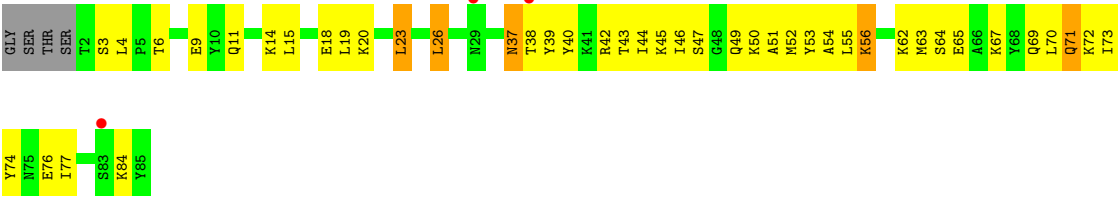
• Molecule 1: Complement C3



- Molecule 2: Complement C3



- Molecule 3: Staphylococcal complement inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.03Å 128.03Å 468.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 7.54 49.62 – 7.54	Depositor EDS
% Data completeness (in resolution range)	86.2 (49.62-7.54) 86.9 (49.62-7.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 7.37Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.265 , 0.268 0.291 , 0.293	Depositor DCC
R_{free} test set	265 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	427.9	Xtriage
Anisotropy	1.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 254.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12785	wwPDB-VP
Average B, all atoms (Å ²)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.56	0/5030	1.00	22/6834 (0.3%)
2	B	0.53	0/7257	0.91	9/9824 (0.1%)
3	M	0.46	0/690	0.89	2/923 (0.2%)
All	All	0.54	0/12977	0.94	33/17581 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	GLN	N-CA-C	-9.31	101.13	111.28
1	A	381	GLY	N-CA-C	-9.27	103.82	115.31
1	A	430	SER	N-CA-C	-7.54	103.06	111.28
1	A	429	ASN	N-CA-C	-7.50	104.60	113.38
1	A	538	VAL	N-CA-C	6.97	117.73	110.62
1	A	21	VAL	N-CA-C	6.76	117.47	106.72
2	B	1033	GLN	N-CA-C	-6.72	105.62	113.88
1	A	537	CYS	N-CA-C	-6.56	100.72	110.23
2	B	1266	ASP	N-CA-C	-6.45	104.59	113.56
2	B	987	GLY	N-CA-C	6.29	119.39	111.85
1	A	609	SER	N-CA-C	6.25	116.49	108.24
2	B	1026	LEU	N-CA-C	-6.21	103.39	111.71
2	B	913	GLY	N-CA-C	6.05	119.62	110.18
2	B	1133	LYS	N-CA-C	6.00	117.82	111.28
1	A	191	SER	CB-CA-C	-5.81	104.41	110.33
1	A	169	LEU	N-CA-C	5.77	117.62	108.79
1	A	64	VAL	N-CA-C	5.74	115.41	108.06
2	B	747	GLU	N-CA-C	5.70	117.57	111.36
1	A	428	GLY	N-CA-C	-5.58	100.56	114.74
1	A	170	SER	N-CA-C	5.56	117.10	107.93
1	A	481	ALA	N-CA-C	5.54	117.27	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	26	LEU	N-CA-C	-5.39	106.67	113.20
1	A	288	GLY	N-CA-C	-5.36	108.30	115.32
1	A	109	PHE	N-CA-C	5.33	118.13	109.06
1	A	320	GLU	N-CA-C	5.29	116.66	107.93
2	B	1182	GLY	CA-C-N	5.29	124.90	119.56
2	B	1182	GLY	C-N-CA	5.29	124.90	119.56
1	A	608	GLY	N-CA-C	5.24	119.01	112.73
1	A	84	VAL	N-CA-C	5.19	115.53	107.28
1	A	55	THR	CA-C-N	-5.09	113.48	119.84
1	A	55	THR	C-N-CA	-5.09	113.48	119.84
3	M	37	ASN	N-CA-C	5.01	117.61	109.79
1	A	382	ASP	N-CA-C	5.01	120.23	113.72

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	4932	0	4999	658	0
2	B	7118	0	7041	702	0
3	M	682	0	697	51	0
4	A	42	0	39	5	0
5	A	11	0	10	1	0
All	All	12785	0	12786	1320	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 57.

All (1320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1269:GLU:O	2:B:1270:LEU:CG	1.69	1.41
1:A:363:TYR:CD1	1:A:364:ARG:HG3	1.60	1.35
1:A:363:TYR:CE1	1:A:364:ARG:HG3	1.60	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:783:LEU:N	2:B:798:PRO:HB3	1.41	1.34
1:A:541:LEU:CG	2:B:796:ALA:HB2	1.62	1.29
1:A:541:LEU:HG	2:B:796:ALA:CB	1.62	1.27
1:A:363:TYR:CA	1:A:379:THR:HG21	1.69	1.21
1:A:516:ILE:HB	1:A:522:ARG:NE	1.56	1.20
1:A:591:GLN:CB	2:B:795:VAL:HG11	1.71	1.19
1:A:380:GLN:NE2	1:A:440:ARG:HH12	1.40	1.18
1:A:363:TYR:HA	1:A:379:THR:CG2	1.72	1.17
2:B:965:VAL:HG13	2:B:1267:HIS:CD2	1.79	1.17
2:B:965:VAL:HG13	2:B:1267:HIS:NE2	1.59	1.15
1:A:363:TYR:CE1	1:A:364:ARG:CG	2.30	1.15
1:A:516:ILE:HB	1:A:522:ARG:CD	1.75	1.15
2:B:782:ILE:C	2:B:798:PRO:CB	2.21	1.14
1:A:591:GLN:HB2	2:B:795:VAL:HG11	1.24	1.14
1:A:515:LEU:HD23	1:A:515:LEU:O	1.49	1.13
2:B:782:ILE:CG2	2:B:783:LEU:H	1.60	1.12
2:B:1361:THR:HB	2:B:1442:HIS:HA	1.32	1.11
2:B:744:GLU:CG	2:B:775:ASP:H	1.65	1.10
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.31	1.10
1:A:591:GLN:HB2	2:B:795:VAL:CG1	1.82	1.09
2:B:782:ILE:C	2:B:798:PRO:HB3	1.76	1.09
2:B:782:ILE:HG22	2:B:783:LEU:N	1.59	1.07
2:B:978:LEU:HD21	2:B:981:LEU:HG	1.33	1.06
1:A:380:GLN:HE22	1:A:440:ARG:NH1	1.53	1.06
2:B:744:GLU:HG3	2:B:775:ASP:H	1.15	1.05
1:A:364:ARG:N	1:A:379:THR:HB	1.70	1.05
1:A:610:GLY:HA3	1:A:616:VAL:HG23	1.36	1.05
1:A:222:TYR:CE1	1:A:328:THR:HG22	1.93	1.04
1:A:302:LEU:HD11	1:A:326:ILE:HD11	1.06	1.02
2:B:799:PHE:O	2:B:800:GLU:HG3	1.58	1.02
1:A:13:ARG:HH22	1:A:476:GLY:HA3	1.25	1.00
2:B:1458:TYR:HB3	2:B:1466:SER:HB3	1.41	0.99
2:B:1128:SER:HA	2:B:1131:GLU:OE2	1.61	0.99
1:A:363:TYR:CE1	1:A:364:ARG:NH1	2.30	0.99
2:B:964:PRO:HB3	2:B:1270:LEU:HD11	1.45	0.97
1:A:501:THR:O	1:A:538:VAL:HG22	1.64	0.97
2:B:783:LEU:N	2:B:798:PRO:CB	2.25	0.97
1:A:364:ARG:H	1:A:379:THR:HB	1.21	0.97
1:A:341:TYR:HB2	1:A:609:SER:HB2	1.48	0.96
2:B:917:ASN:HB3	2:B:1325:MET:HE2	1.44	0.96
1:A:478:LEU:HD21	1:A:622:LEU:HD21	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:833:ARG:HH11	2:B:833:ARG:HG2	1.29	0.96
2:B:1269:GLU:O	2:B:1270:LEU:HG	0.78	0.95
1:A:554:VAL:HG12	1:A:555:PRO:HD2	1.47	0.95
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.47	0.95
2:B:799:PHE:HD1	2:B:800:GLU:H	1.10	0.95
1:A:516:ILE:HB	1:A:522:ARG:HE	1.18	0.95
1:A:567:HIS:CG	2:B:760:PRO:HG3	2.00	0.95
2:B:1397:LYS:NZ	2:B:1412:LEU:HG	1.80	0.95
1:A:591:GLN:CB	2:B:795:VAL:CG1	2.44	0.95
1:A:430:SER:O	1:A:431:ASN:CG	2.09	0.95
1:A:589:LEU:HD11	1:A:594:ILE:HD11	1.49	0.94
1:A:590:THR:HB	1:A:593:LYS:HG3	1.48	0.94
2:B:972:ALA:HB1	2:B:1005:TYR:OH	1.66	0.94
1:A:302:LEU:CD1	1:A:326:ILE:HD11	1.96	0.94
1:A:541:LEU:HG	2:B:796:ALA:HB2	0.94	0.94
2:B:914:ILE:HG23	2:B:1328:ALA:HB3	1.49	0.94
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.47	0.94
2:B:1269:GLU:C	2:B:1270:LEU:HG	1.92	0.93
2:B:965:VAL:CG1	2:B:1267:HIS:NE2	2.30	0.93
1:A:515:LEU:HD23	1:A:515:LEU:C	1.93	0.92
2:B:965:VAL:C	2:B:1267:HIS:HD2	1.76	0.92
1:A:377:SER:OG	1:A:387:LEU:HG	1.68	0.92
2:B:1268:GLN:O	2:B:1268:GLN:HG2	1.69	0.92
2:B:1278:LEU:H	2:B:1281:ARG:HD2	1.34	0.92
1:A:327:VAL:HG21	1:A:357:PRO:HB3	1.47	0.92
1:A:36:THR:HG23	1:A:48:SER:HB3	1.50	0.91
2:B:965:VAL:O	2:B:1267:HIS:CD2	2.24	0.91
1:A:363:TYR:CD1	1:A:364:ARG:CG	2.51	0.91
2:B:799:PHE:CD1	2:B:800:GLU:N	2.37	0.91
2:B:783:LEU:HA	2:B:798:PRO:HD3	1.49	0.91
2:B:1259:GLN:HE22	2:B:1262:LYS:HE2	1.34	0.91
1:A:339:PRO:HA	1:A:608:GLY:HA3	1.52	0.91
1:A:363:TYR:HA	1:A:379:THR:HG21	0.90	0.90
2:B:1055:TRP:CE2	2:B:1108:ILE:HG22	2.07	0.90
1:A:113:ASP:HB2	2:B:751:TRP:CZ3	2.07	0.90
2:B:745:PHE:N	2:B:746:PRO:HD2	1.87	0.90
1:A:246:THR:HB	2:B:1425:TYR:OH	1.72	0.89
1:A:328:THR:O	1:A:330:PRO:HD3	1.72	0.89
1:A:522:ARG:HH11	1:A:522:ARG:CG	1.84	0.89
1:A:207:LEU:HD21	2:B:747:GLU:HG2	1.51	0.89
1:A:516:ILE:HD12	1:A:522:ARG:HD3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:736:GLU:HG2	2:B:891:LYS:HD2	1.55	0.88
1:A:220:PHE:CZ	1:A:330:PRO:HB3	2.08	0.88
2:B:1397:LYS:HZ3	2:B:1412:LEU:HG	1.38	0.88
2:B:782:ILE:HG22	2:B:783:LEU:H	0.74	0.88
2:B:978:LEU:HD11	2:B:981:LEU:HD12	1.55	0.88
1:A:363:TYR:HE1	1:A:364:ARG:HD3	1.38	0.87
2:B:1126:LEU:HD23	2:B:1173:ALA:HB1	1.56	0.87
1:A:543:VAL:HG12	2:B:799:PHE:HE2	1.38	0.86
2:B:744:GLU:HG3	2:B:775:ASP:N	1.90	0.86
2:B:992:ASN:HD21	2:B:1033:GLN:HB2	1.40	0.86
1:A:220:PHE:CG	1:A:357:PRO:HG2	2.10	0.86
1:A:459:ARG:O	1:A:459:ARG:HG3	1.74	0.86
1:A:555:PRO:HB3	2:B:775:ASP:HA	1.56	0.86
1:A:591:GLN:O	1:A:594:ILE:HB	1.75	0.86
2:B:965:VAL:O	2:B:1267:HIS:HD2	1.55	0.86
2:B:964:PRO:CB	2:B:1270:LEU:HD11	2.06	0.86
2:B:1168:ALA:HA	2:B:1188:PHE:HE1	1.40	0.85
1:A:363:TYR:HE1	1:A:364:ARG:CD	1.87	0.85
2:B:809:ILE:O	2:B:903:VAL:HG21	1.75	0.85
1:A:248:PHE:HD1	2:B:1378:MET:HE3	1.40	0.85
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.12	0.85
2:B:756:LEU:HD13	2:B:765:SER:HB2	1.59	0.84
2:B:783:LEU:HB2	2:B:798:PRO:HG3	1.58	0.84
1:A:537:CYS:HB2	2:B:794:CYS:HA	1.60	0.84
1:A:253:ILE:HB	1:A:260:ILE:HB	1.59	0.84
1:A:364:ARG:N	1:A:379:THR:CB	2.40	0.83
2:B:833:ARG:HH22	2:B:899:ILE:HD11	1.43	0.83
1:A:472:ILE:HG21	1:A:503:PHE:CE1	2.14	0.83
1:A:223:ILE:HD13	1:A:328:THR:OG1	1.79	0.83
1:A:591:GLN:HG2	2:B:795:VAL:HG12	1.61	0.83
1:A:107:TYR:HB2	1:A:109:PHE:CZ	2.13	0.83
2:B:799:PHE:O	2:B:800:GLU:CG	2.27	0.83
1:A:8:THR:CG2	1:A:20:MET:HB2	2.08	0.82
1:A:410:SER:O	1:A:414:GLN:HG2	1.79	0.82
1:A:477:ARG:HH11	1:A:477:ARG:CG	1.92	0.82
1:A:363:TYR:CE1	1:A:364:ARG:CD	2.61	0.82
1:A:364:ARG:H	1:A:379:THR:CB	1.93	0.82
2:B:733:ILE:HG12	2:B:734:ILE:H	1.43	0.82
1:A:314:SER:HB3	2:B:812:ARG:HD3	1.60	0.81
2:B:742:ARG:HB2	2:B:903:VAL:HG22	1.59	0.81
1:A:370:GLN:HE22	1:A:403:ARG:NE	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:744:GLU:C	2:B:746:PRO:HD2	2.03	0.81
1:A:378:LEU:HD13	1:A:379:THR:N	1.94	0.81
1:A:8:THR:HG23	1:A:20:MET:HB2	1.62	0.81
1:A:369:VAL:HG23	1:A:375:VAL:HG11	1.62	0.81
1:A:516:ILE:HB	1:A:522:ARG:HD2	1.63	0.81
2:B:882:LYS:HE2	2:B:886:GLN:HE22	1.44	0.81
1:A:553:PRO:HB2	2:B:773:LEU:HD12	1.63	0.80
1:A:522:ARG:HH11	1:A:522:ARG:HG3	1.45	0.80
1:A:327:VAL:HG21	1:A:357:PRO:CB	2.11	0.80
1:A:430:SER:O	1:A:431:ASN:CB	2.30	0.80
2:B:966:ALA:HA	2:B:1267:HIS:HB3	1.61	0.80
1:A:363:TYR:CD1	1:A:364:ARG:NH1	2.49	0.80
1:A:440:ARG:HG3	1:A:440:ARG:O	1.81	0.80
2:B:745:PHE:N	2:B:746:PRO:CD	2.44	0.80
2:B:782:ILE:HD12	2:B:799:PHE:CE2	2.16	0.80
2:B:1193:LYS:HD3	2:B:1199:GLU:OE2	1.81	0.80
1:A:380:GLN:CD	1:A:384:VAL:O	2.24	0.80
1:A:591:GLN:HA	1:A:594:ILE:CG1	2.13	0.79
1:A:516:ILE:CB	1:A:522:ARG:CD	2.59	0.79
1:A:522:ARG:HG3	1:A:522:ARG:NH1	1.96	0.79
1:A:591:GLN:HB3	2:B:795:VAL:HG11	1.64	0.79
1:A:469:THR:HB	1:A:512:TYR:CE2	2.18	0.79
1:A:6:ILE:HD11	1:A:20:MET:HG2	1.65	0.79
1:A:97:LYS:HG3	1:A:98:VAL:N	1.98	0.79
1:A:13:ARG:HH22	1:A:476:GLY:CA	1.96	0.78
1:A:378:LEU:HD13	1:A:378:LEU:C	2.08	0.78
1:A:624:PHE:HB3	1:A:632:THR:HG23	1.64	0.78
1:A:501:THR:O	1:A:538:VAL:CG2	2.31	0.78
1:A:541:LEU:CD2	2:B:796:ALA:HB2	2.12	0.78
1:A:14:LEU:HD21	1:A:101:VAL:CG1	2.14	0.78
1:A:509:LEU:C	1:A:509:LEU:HD13	2.09	0.78
1:A:528:SER:HB3	1:A:616:VAL:HG13	1.65	0.78
2:B:1369:ARG:HD3	2:B:1434:ASP:OD1	1.83	0.78
2:B:1228:PRO:HB2	2:B:1229:PRO:CD	2.12	0.78
1:A:351:MET:HE1	1:A:386:LYS:HE3	1.66	0.77
1:A:329:SER:OG	1:A:415:ALA:HB2	1.84	0.77
1:A:341:TYR:CE1	1:A:611:LYS:HG3	2.19	0.77
1:A:327:VAL:CG2	1:A:357:PRO:HB3	2.13	0.77
1:A:380:GLN:HE22	1:A:440:ARG:HH12	0.79	0.77
2:B:1130:GLN:NE2	2:B:1177:MET:HE2	1.99	0.77
2:B:1277:GLN:C	2:B:1278:LEU:HD12	2.09	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ILE:CB	1:A:522:ARG:HE	1.96	0.77
1:A:501:THR:OG1	1:A:538:VAL:HG13	1.85	0.77
2:B:783:LEU:HA	2:B:798:PRO:CD	2.14	0.77
2:B:1038:ARG:CD	2:B:1077:VAL:HG13	2.15	0.77
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.67	0.76
1:A:363:TYR:HE1	1:A:364:ARG:HH11	1.26	0.76
1:A:470:TYR:C	1:A:471:LEU:HD12	2.10	0.76
1:A:221:TYR:CE1	1:A:228:GLY:HA2	2.21	0.76
1:A:591:GLN:HB2	2:B:795:VAL:CB	2.15	0.76
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	1.68	0.76
2:B:1259:GLN:HE22	2:B:1262:LYS:CE	1.97	0.76
1:A:113:ASP:OD1	1:A:114:LYS:HG3	1.85	0.76
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.68	0.76
2:B:782:ILE:HB	2:B:798:PRO:CB	2.16	0.76
2:B:1086:ILE:HD13	2:B:1142:SER:O	1.86	0.75
1:A:590:THR:HG22	1:A:592:SER:N	2.00	0.75
2:B:1259:GLN:HE22	2:B:1262:LYS:HB2	1.51	0.75
1:A:6:ILE:HD12	1:A:7:ILE:H	1.50	0.75
2:B:993:MET:HE3	2:B:1059:TYR:CE2	2.20	0.75
1:A:131:ASN:HD21	1:A:133:LYS:HD3	1.52	0.75
1:A:142:MET:SD	1:A:189:GLU:HB2	2.28	0.74
2:B:960:LEU:HB2	2:B:1298:ARG:O	1.86	0.74
1:A:220:PHE:CB	1:A:357:PRO:HG2	2.17	0.74
2:B:1396:LEU:HD22	2:B:1407:ILE:CD1	2.17	0.74
2:B:783:LEU:H	2:B:798:PRO:HB3	1.52	0.74
2:B:957:ARG:HG3	2:B:1301:GLU:CG	2.17	0.74
2:B:1342:LYS:HE3	2:B:1367:CYS:HB3	1.69	0.73
1:A:614:ALA:HB1	1:A:632:THR:HA	1.69	0.73
1:A:610:GLY:HA3	1:A:616:VAL:CG2	2.17	0.73
2:B:1084:TRP:CD1	2:B:1088:GLU:HG3	2.23	0.73
1:A:451:VAL:HB	1:A:495:LEU:HB3	1.71	0.73
1:A:556:GLY:O	3:M:39:TYR:HB2	1.87	0.73
1:A:562:LYS:O	1:A:563:ILE:HG13	1.88	0.73
1:A:590:THR:O	1:A:594:ILE:HG12	1.88	0.73
2:B:964:PRO:CG	2:B:1270:LEU:HD11	2.19	0.73
1:A:516:ILE:CB	1:A:522:ARG:HD2	2.19	0.72
2:B:883:THR:HG21	2:B:911:PRO:HG3	1.69	0.72
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.72	0.72
1:A:439:LEU:H	1:A:439:LEU:HD12	1.53	0.72
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.71	0.72
1:A:404:THR:HG23	1:A:414:GLN:HE21	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1396:LEU:HD22	2:B:1407:ILE:HD13	1.72	0.72
2:B:978:LEU:HD11	2:B:981:LEU:CD1	2.19	0.72
1:A:114:LYS:HD2	2:B:747:GLU:OE1	1.90	0.72
1:A:216:PRO:HG3	1:A:231:VAL:HG22	1.71	0.72
2:B:833:ARG:HH11	2:B:833:ARG:CG	2.02	0.72
1:A:19:THR:HG22	1:A:20:MET:H	1.53	0.71
2:B:744:GLU:HB2	2:B:775:ASP:HB2	1.71	0.71
2:B:782:ILE:O	2:B:798:PRO:HG3	1.90	0.71
1:A:10:ASN:HB2	1:A:621:GLY:C	2.15	0.71
1:A:40:PHE:HD1	1:A:85:THR:OG1	1.74	0.71
1:A:97:LYS:HG3	1:A:98:VAL:H	1.54	0.71
1:A:427:VAL:CG2	1:A:613:TYR:CE2	2.72	0.71
2:B:782:ILE:O	2:B:783:LEU:HB2	1.90	0.71
2:B:934:GLY:O	2:B:935:VAL:HG22	1.90	0.71
2:B:964:PRO:HB3	2:B:1270:LEU:CD1	2.19	0.71
1:A:530:TRP:CG	1:A:607:PRO:HB3	2.25	0.71
1:A:40:PHE:HD1	1:A:85:THR:HG1	1.38	0.71
2:B:996:MET:HE1	2:B:1030:GLY:HA3	1.71	0.71
2:B:1334:LEU:HD12	2:B:1336:CYS:H	1.56	0.71
3:M:3:SER:O	3:M:4:LEU:HG	1.90	0.71
1:A:504:ILE:HG21	1:A:536:SER:H	1.54	0.71
1:A:312:SER:HB2	2:B:873:SER:HB2	1.71	0.71
1:A:369:VAL:CG2	1:A:375:VAL:HG11	2.21	0.70
1:A:577:ASP:OD1	2:B:778:THR:HG21	1.90	0.70
2:B:964:PRO:HG3	2:B:1270:LEU:HD11	1.74	0.70
3:M:49:GLN:HA	3:M:52:MET:HE2	1.70	0.70
1:A:251:PHE:HD2	1:A:265:SER:HB2	1.56	0.70
1:A:327:VAL:HG21	1:A:357:PRO:CG	2.21	0.70
2:B:782:ILE:C	2:B:798:PRO:HB2	2.16	0.70
2:B:994:ILE:HG23	2:B:1247:THR:OG1	1.91	0.70
2:B:1090:GLN:HE22	2:B:1146:SER:HA	1.54	0.70
2:B:782:ILE:C	2:B:798:PRO:CG	2.65	0.70
1:A:14:LEU:HD21	1:A:101:VAL:HG13	1.74	0.70
1:A:530:TRP:CE3	1:A:607:PRO:HB2	2.27	0.70
1:A:567:HIS:CD2	2:B:760:PRO:HG3	2.25	0.70
1:A:574:VAL:HB	2:B:751:TRP:CE3	2.27	0.70
2:B:956:THR:OG1	2:B:1324:THR:HG22	1.91	0.70
1:A:179:MET:HG3	1:A:202:VAL:O	1.91	0.70
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.72	0.70
1:A:26:ASP:OD2	1:A:522:ARG:NH2	2.24	0.70
1:A:314:SER:CB	2:B:812:ARG:HD3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:740:VAL:HB	3:M:42:ARG:HB2	1.73	0.70
1:A:339:PRO:CA	1:A:608:GLY:HA3	2.20	0.70
2:B:749:TRP:CE3	2:B:750:LEU:HB2	2.27	0.70
1:A:590:THR:HG22	1:A:592:SER:H	1.55	0.70
2:B:1055:TRP:CD2	2:B:1108:ILE:HG22	2.27	0.70
1:A:125:TYR:OH	1:A:145:ILE:HD11	1.91	0.69
1:A:210:PHE:O	1:A:582:VAL:HG11	1.91	0.69
2:B:1041:SER:HG	2:B:1084:TRP:CG	2.09	0.69
1:A:221:TYR:HB3	1:A:326:ILE:HD13	1.73	0.69
1:A:7:ILE:HG22	1:A:8:THR:H	1.56	0.69
1:A:114:LYS:HE3	1:A:117:TYR:CD1	2.27	0.69
2:B:744:GLU:CB	2:B:775:ASP:H	2.05	0.69
1:A:309:ILE:HG12	1:A:316:MET:HB2	1.74	0.69
2:B:903:VAL:HG12	2:B:905:LYS:HG3	1.74	0.69
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	1.75	0.69
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.74	0.69
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.23	0.68
1:A:3:MET:HE2	1:A:5:SER:HB3	1.76	0.68
2:B:783:LEU:CB	2:B:798:PRO:HG3	2.22	0.68
2:B:1365:GLU:HG3	2:B:1438:ALA:HB2	1.74	0.68
1:A:471:LEU:O	1:A:509:LEU:CD2	2.41	0.68
1:A:501:THR:HB	1:A:538:VAL:HG22	1.74	0.68
2:B:749:TRP:HB2	2:B:774:LYS:HE2	1.75	0.68
2:B:1416:PHE:HZ	2:B:1442:HIS:HD2	1.41	0.68
1:A:158:LEU:HG	1:A:159:SER:H	1.58	0.68
1:A:222:TYR:CE1	1:A:328:THR:CG2	2.75	0.68
1:A:5:SER:HA	1:A:626:SER:HA	1.75	0.68
2:B:757:LYS:HA	2:B:757:LYS:CE	2.24	0.68
2:B:914:ILE:CG2	2:B:1328:ALA:HB3	2.21	0.68
2:B:1084:TRP:O	2:B:1088:GLU:HB2	1.93	0.68
1:A:168:PRO:O	1:A:169:LEU:HD23	1.93	0.68
2:B:1475:LYS:H	2:B:1475:LYS:HD2	1.59	0.68
3:M:50:LYS:HE2	3:M:65:GLU:HG3	1.76	0.68
4:A:647:NAG:H61	5:A:648:MAN:C1	2.23	0.67
2:B:829:LEU:HD23	2:B:840:VAL:HG11	1.75	0.67
2:B:850:PHE:CE1	2:B:886:GLN:HB3	2.28	0.67
2:B:783:LEU:CA	2:B:798:PRO:HG3	2.25	0.67
2:B:1278:LEU:N	2:B:1281:ARG:HD2	2.09	0.67
2:B:957:ARG:HG3	2:B:1301:GLU:HG3	1.76	0.67
1:A:378:LEU:CD1	1:A:379:THR:O	2.42	0.67
1:A:590:THR:CG2	1:A:592:SER:HB3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1406:TYR:CZ	2:B:1408:SER:HA	2.29	0.67
2:B:809:ILE:HG21	2:B:890:VAL:HG23	1.77	0.67
2:B:866:ILE:HG12	2:B:872:LEU:CD2	2.24	0.67
2:B:750:LEU:HD12	2:B:752:ASN:OD1	1.94	0.67
1:A:592:SER:O	1:A:596:ASP:HB2	1.95	0.67
2:B:850:PHE:CZ	2:B:886:GLN:HB3	2.30	0.66
2:B:795:VAL:HG13	2:B:795:VAL:O	1.94	0.66
2:B:1259:GLN:NE2	2:B:1262:LYS:HB2	2.09	0.66
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.30	0.66
1:A:117:TYR:CZ	1:A:123:VAL:HG13	2.31	0.66
1:A:591:GLN:CG	2:B:795:VAL:CG1	2.74	0.66
2:B:739:ILE:HG12	2:B:900:SER:HB2	1.78	0.66
2:B:805:GLN:HG2	2:B:806:ASP:H	1.60	0.66
2:B:975:ALA:CB	2:B:1006:LEU:HD21	2.26	0.66
1:A:433:TYR:HD2	1:A:456:ARG:HG2	1.60	0.66
2:B:964:PRO:HB2	2:B:1291:TRP:HZ3	1.61	0.66
2:B:964:PRO:HB2	2:B:1291:TRP:CZ3	2.30	0.66
1:A:221:TYR:HE1	1:A:228:GLY:HA2	1.60	0.66
2:B:744:GLU:OE1	2:B:774:LYS:HD2	1.96	0.66
1:A:591:GLN:HA	1:A:594:ILE:HG12	1.78	0.65
2:B:1342:LYS:HB2	2:B:1367:CYS:HB2	1.78	0.65
1:A:370:GLN:HE22	1:A:403:ARG:HE	1.42	0.65
2:B:1219:LEU:HD21	2:B:1227:VAL:HG11	1.78	0.65
2:B:1168:ALA:HA	2:B:1188:PHE:CE1	2.28	0.65
1:A:335:PHE:CE2	1:A:417:ARG:HG3	2.31	0.65
2:B:782:ILE:CB	2:B:798:PRO:HB3	2.25	0.65
2:B:1046:ALA:N	2:B:1056:LEU:HD23	2.10	0.65
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.62	0.65
1:A:576:VAL:HG11	1:A:581:PHE:CZ	2.31	0.65
1:A:125:TYR:CE1	1:A:169:LEU:HD13	2.31	0.65
1:A:222:TYR:HE1	1:A:328:THR:HG22	1.60	0.65
1:A:248:PHE:CD1	2:B:1378:MET:HE3	2.27	0.65
1:A:364:ARG:CA	1:A:379:THR:HB	2.27	0.65
1:A:554:VAL:HG12	1:A:555:PRO:CD	2.26	0.65
1:A:325:PRO:HG2	1:A:357:PRO:C	2.21	0.65
2:B:1259:GLN:NE2	2:B:1262:LYS:HE2	2.11	0.65
1:A:55:THR:HB	1:A:57:ALA:H	1.62	0.65
1:A:445:PRO:HG3	1:A:504:ILE:HD11	1.77	0.65
2:B:1192:ALA:HB2	2:B:1198:TRP:CH2	2.31	0.65
2:B:1279:PRO:HG2	2:B:1306:GLU:HB3	1.77	0.65
1:A:224:TYR:HE2	1:A:328:THR:HG21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1277:GLN:HG3	2:B:1281:ARG:HE	1.60	0.65
2:B:1166:THR:HA	2:B:1169:ILE:HG22	1.78	0.65
1:A:129:THR:O	1:A:130:VAL:HG13	1.98	0.64
1:A:378:LEU:HD13	1:A:379:THR:O	1.97	0.64
1:A:590:THR:HB	1:A:593:LYS:CG	2.24	0.64
1:A:472:ILE:HG21	1:A:503:PHE:HE1	1.62	0.64
2:B:757:LYS:HA	2:B:757:LYS:HE2	1.79	0.64
3:M:53:TYR:CD1	3:M:56:LYS:HE2	2.33	0.64
2:B:843:GLU:HB2	2:B:861:GLN:HB3	1.78	0.64
2:B:866:ILE:HG12	2:B:872:LEU:HD23	1.79	0.64
1:A:386:LYS:HD3	1:A:440:ARG:HD3	1.80	0.64
1:A:471:LEU:O	1:A:509:LEU:HD22	1.98	0.64
2:B:964:PRO:HB3	2:B:1270:LEU:HD21	1.79	0.64
1:A:13:ARG:O	1:A:14:LEU:HD23	1.98	0.64
1:A:591:GLN:CG	2:B:795:VAL:HG12	2.27	0.64
2:B:782:ILE:CB	2:B:798:PRO:CB	2.76	0.64
1:A:342:PHE:CE1	1:A:391:THR:HG21	2.32	0.64
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.61	0.64
2:B:1128:SER:O	2:B:1129:LEU:HD23	1.98	0.63
2:B:1180:LEU:O	2:B:1185:LEU:HB2	1.98	0.63
2:B:782:ILE:CD1	2:B:799:PHE:CE2	2.81	0.63
1:A:427:VAL:C	1:A:429:ASN:H	2.06	0.63
1:A:591:GLN:HA	1:A:594:ILE:HG13	1.80	0.63
2:B:954:SER:HB2	2:B:1326:TYR:HB3	1.81	0.63
2:B:996:MET:CE	2:B:1030:GLY:HA3	2.29	0.63
2:B:813:LEU:HD22	2:B:905:LYS:HB2	1.80	0.63
1:A:380:GLN:CG	1:A:384:VAL:O	2.46	0.63
1:A:591:GLN:HG2	2:B:795:VAL:CG1	2.29	0.63
1:A:605:CYS:O	1:A:607:PRO:HD3	1.98	0.63
2:B:978:LEU:C	2:B:978:LEU:HD22	2.24	0.63
2:B:1039:GLN:HE21	2:B:1048:VAL:HA	1.63	0.63
1:A:504:ILE:HD13	1:A:536:SER:OG	1.98	0.62
1:A:590:THR:HG21	1:A:592:SER:HB3	1.79	0.62
2:B:1366:ILE:HD13	2:B:1455:VAL:HG11	1.81	0.62
1:A:135:LEU:HB3	1:A:136:PRO:HD2	1.81	0.62
2:B:957:ARG:HG3	2:B:1301:GLU:HG2	1.79	0.62
2:B:782:ILE:C	2:B:798:PRO:HG3	2.25	0.62
2:B:998:PRO:O	2:B:1001:ILE:HG22	1.99	0.62
1:A:6:ILE:HD12	1:A:7:ILE:N	2.14	0.62
1:A:22:LEU:O	1:A:23:GLU:HG3	2.00	0.62
2:B:985:PRO:HD2	2:B:1026:LEU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1254:PHE:O	2:B:1258:ALA:N	2.32	0.62
2:B:1472:HIS:HB2	2:B:1478:GLY:HA2	1.80	0.62
2:B:782:ILE:CG2	2:B:783:LEU:N	2.34	0.62
2:B:1228:PRO:CB	2:B:1229:PRO:HD3	2.17	0.62
2:B:782:ILE:O	2:B:783:LEU:CB	2.48	0.62
2:B:1039:GLN:HB3	2:B:1040:PRO:HD2	1.80	0.62
2:B:1130:GLN:CD	2:B:1177:MET:HE2	2.24	0.62
1:A:130:VAL:HG12	1:A:135:LEU:O	1.99	0.62
1:A:187:TYR:HB3	1:A:195:VAL:HG22	1.80	0.62
2:B:965:VAL:CG1	2:B:1267:HIS:CD2	2.72	0.62
1:A:363:TYR:C	1:A:379:THR:HG21	2.25	0.62
2:B:1056:LEU:O	2:B:1056:LEU:HG	1.98	0.62
2:B:1237:GLN:OE1	2:B:1237:GLN:HA	2.00	0.62
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.35	0.61
1:A:477:ARG:HH11	1:A:477:ARG:HG2	1.65	0.61
2:B:782:ILE:CA	2:B:798:PRO:HB2	2.30	0.61
2:B:1227:VAL:N	2:B:1228:PRO:HD2	2.15	0.61
1:A:216:PRO:HA	1:A:231:VAL:HA	1.82	0.61
1:A:580:VAL:CG2	2:B:747:GLU:HB3	2.29	0.61
2:B:1342:LYS:HE3	2:B:1367:CYS:CB	2.31	0.61
1:A:186:ALA:O	1:A:195:VAL:HG13	2.00	0.61
2:B:782:ILE:CA	2:B:798:PRO:CB	2.78	0.61
2:B:783:LEU:CA	2:B:798:PRO:CG	2.78	0.61
2:B:1381:LEU:HD11	2:B:1426:LEU:HD11	1.82	0.61
2:B:1390:ALA:HB2	2:B:1444:TYR:CE2	2.35	0.61
1:A:377:SER:HG	1:A:387:LEU:HG	1.65	0.61
2:B:1098:GLU:OE2	2:B:1101:PRO:HA	2.00	0.61
2:B:1219:LEU:CD2	2:B:1227:VAL:HG21	2.30	0.61
1:A:251:PHE:CD2	1:A:265:SER:HB2	2.35	0.61
2:B:1265:PRO:O	2:B:1266:ASP:HB2	2.00	0.61
3:M:53:TYR:HA	3:M:56:LYS:HG2	1.82	0.61
1:A:144:ASN:CG	1:A:155:GLN:HE21	2.08	0.61
1:A:137:VAL:HG22	1:A:139:ARG:NH1	2.14	0.61
2:B:1128:SER:HA	2:B:1131:GLU:CD	2.25	0.61
1:A:158:LEU:HG	1:A:159:SER:N	2.15	0.61
1:A:222:TYR:HB3	1:A:225:ASN:HB2	1.83	0.61
2:B:819:ARG:O	2:B:820:ASN:HB2	2.01	0.61
2:B:1187:LYS:O	2:B:1187:LYS:HG2	2.01	0.61
2:B:1205:LEU:HD22	2:B:1249:ALA:CB	2.30	0.61
2:B:1278:LEU:O	2:B:1281:ARG:HD3	2.00	0.61
1:A:221:TYR:HB3	1:A:326:ILE:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:738:ASN:HD22	3:M:45:LYS:HB3	1.65	0.60
1:A:32:PRO:HA	1:A:53:VAL:HG22	1.83	0.60
1:A:114:LYS:HB2	1:A:117:TYR:CE1	2.36	0.60
1:A:224:TYR:CE2	1:A:328:THR:HG21	2.36	0.60
2:B:1047:PHE:HB2	2:B:1050:ARG:HB3	1.82	0.60
2:B:1396:LEU:O	2:B:1407:ILE:HD12	2.01	0.60
1:A:13:ARG:NH2	1:A:476:GLY:HA3	2.08	0.60
1:A:365:VAL:HG12	1:A:379:THR:OG1	2.01	0.60
1:A:365:VAL:HG23	1:A:406:LYS:HB2	1.83	0.60
1:A:509:LEU:HD22	1:A:510:VAL:N	2.15	0.60
1:A:543:VAL:HG12	2:B:799:PHE:CE2	2.28	0.60
1:A:13:ARG:C	1:A:14:LEU:HD23	2.25	0.60
1:A:142:MET:HG3	1:A:187:TYR:CZ	2.36	0.60
1:A:566:ASP:O	2:B:756:LEU:HD12	2.02	0.60
2:B:851:CYS:O	2:B:851:CYS:SG	2.58	0.60
2:B:1012:TRP:CZ3	2:B:1020:ARG:HB2	2.36	0.60
2:B:1192:ALA:CB	2:B:1195:LYS:HA	2.32	0.60
2:B:1370:TYR:CD2	2:B:1376:ALA:HB2	2.37	0.60
1:A:361:PRO:HB2	1:A:383:GLY:HA3	1.84	0.60
1:A:508:ARG:CZ	1:A:604:GLY:HA3	2.31	0.60
2:B:974:ASP:C	2:B:976:GLU:N	2.57	0.60
1:A:7:ILE:HG22	1:A:8:THR:N	2.16	0.60
1:A:477:ARG:CZ	1:A:479:LEU:HD13	2.32	0.60
1:A:147:ASN:HA	1:A:182:TRP:CE3	2.37	0.59
2:B:1259:GLN:HE22	2:B:1262:LYS:CB	2.15	0.59
1:A:107:TYR:CB	1:A:109:PHE:CZ	2.84	0.59
2:B:993:MET:HE3	2:B:1059:TYR:CD2	2.36	0.59
2:B:1086:ILE:HG23	2:B:1146:SER:HB2	1.84	0.59
1:A:78:LYS:HD3	1:A:82:LYS:HE3	1.83	0.59
2:B:1338:LYS:CA	2:B:1371:ARG:HB2	2.26	0.59
2:B:1459:ALA:HB1	2:B:1461:TYR:CE2	2.37	0.59
1:A:9:PRO:HG2	1:A:18:GLU:OE1	2.02	0.59
2:B:1192:ALA:HB2	2:B:1198:TRP:CZ2	2.37	0.59
1:A:404:THR:HG22	1:A:415:ALA:O	2.01	0.59
1:A:15:GLU:OE1	1:A:190:ASN:ND2	2.33	0.59
1:A:335:PHE:CD2	1:A:417:ARG:HG3	2.37	0.59
1:A:453:PHE:CD2	1:A:493:VAL:O	2.56	0.59
1:A:591:GLN:O	1:A:594:ILE:CB	2.49	0.59
2:B:783:LEU:HA	2:B:798:PRO:CG	2.32	0.59
2:B:1215:LEU:HD11	2:B:1227:VAL:HG13	1.85	0.59
2:B:1038:ARG:O	2:B:1039:GLN:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1123:ALA:HB1	2:B:1169:ILE:O	2.02	0.59
2:B:1269:GLU:O	2:B:1270:LEU:CB	2.45	0.59
1:A:407:GLN:O	1:A:408:GLU:HB2	2.02	0.59
2:B:1038:ARG:NE	2:B:1077:VAL:HG13	2.17	0.59
2:B:1074:ASP:HB3	2:B:1077:VAL:HG23	1.85	0.59
2:B:750:LEU:HG	2:B:750:LEU:O	2.01	0.59
2:B:1205:LEU:HD22	2:B:1249:ALA:HB1	1.85	0.59
2:B:882:LYS:HE2	2:B:886:GLN:NE2	2.17	0.59
2:B:935:VAL:HG23	2:B:935:VAL:O	2.03	0.59
2:B:1181:LYS:HB2	2:B:1181:LYS:NZ	2.18	0.59
2:B:1239:TYR:HE2	2:B:1249:ALA:O	1.86	0.59
1:A:331:TYR:O	1:A:415:ALA:HB3	2.03	0.58
2:B:956:THR:HA	2:B:1324:THR:HA	1.84	0.58
2:B:974:ASP:HB3	2:B:976:GLU:HB2	1.85	0.58
1:A:327:VAL:CG2	1:A:357:PRO:CG	2.81	0.58
1:A:378:LEU:C	1:A:378:LEU:CD1	2.76	0.58
2:B:1270:LEU:HA	2:B:1316:GLY:HA3	1.85	0.58
1:A:152:PRO:HB3	1:A:155:GLN:HE22	1.68	0.58
1:A:380:GLN:C	1:A:382:ASP:H	2.11	0.58
2:B:1416:PHE:CZ	2:B:1442:HIS:HD2	2.22	0.58
1:A:439:LEU:H	1:A:439:LEU:CD1	2.17	0.58
2:B:850:PHE:CZ	2:B:886:GLN:CB	2.86	0.58
2:B:1263:ASP:O	2:B:1264:ALA:C	2.47	0.58
1:A:250:ILE:HD12	2:B:1460:TYR:OH	2.04	0.58
1:A:507:PHE:HE1	1:A:533:VAL:HG23	1.67	0.58
2:B:1087:LEU:HD21	2:B:1142:SER:HB3	1.85	0.58
2:B:1251:PHE:HD1	2:B:1252:MET:SD	2.26	0.58
1:A:103:LEU:HG	1:A:193:GLN:HE21	1.69	0.58
1:A:341:TYR:N	1:A:609:SER:OG	2.37	0.58
2:B:1338:LYS:HA	2:B:1371:ARG:CB	2.30	0.58
1:A:439:LEU:HD12	1:A:439:LEU:N	2.19	0.58
2:B:809:ILE:HG21	2:B:890:VAL:CG2	2.34	0.58
2:B:1227:VAL:N	2:B:1228:PRO:CD	2.67	0.57
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.38	0.57
1:A:179:MET:HG2	1:A:203:LYS:HA	1.85	0.57
1:A:403:ARG:HA	1:A:416:THR:HG22	1.87	0.57
1:A:470:TYR:C	1:A:470:TYR:CD1	2.81	0.57
1:A:517:GLY:O	1:A:518:ALA:HB3	2.04	0.57
2:B:1086:ILE:HG21	2:B:1142:SER:O	2.05	0.57
2:B:965:VAL:C	2:B:1267:HIS:CD2	2.68	0.57
1:A:24:ALA:O	1:A:60:HIS:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:908:LYS:O	2:B:910:VAL:HG23	2.05	0.57
2:B:1155:GLU:HG3	2:B:1184:LEU:HD21	1.85	0.57
1:A:363:TYR:CD2	1:A:381:GLY:HA2	2.39	0.57
1:A:133:LYS:HE3	1:A:477:ARG:CD	2.34	0.57
2:B:739:ILE:HB	2:B:891:LYS:HD3	1.87	0.57
2:B:799:PHE:CE1	2:B:801:VAL:HG23	2.40	0.57
2:B:991:GLN:HE22	2:B:1104:HIS:CE1	2.22	0.57
1:A:410:SER:C	1:A:412:ALA:H	2.12	0.57
1:A:530:TRP:CB	1:A:607:PRO:HB3	2.35	0.57
1:A:553:PRO:HB2	2:B:773:LEU:CD1	2.32	0.57
2:B:828:VAL:HB	2:B:830:TYR:CE2	2.39	0.57
2:B:984:THR:HG23	2:B:1026:LEU:HD22	1.85	0.57
2:B:1403:VAL:HG22	2:B:1404:ASP:H	1.70	0.57
1:A:187:TYR:CB	1:A:195:VAL:HG22	2.35	0.57
1:A:471:LEU:O	1:A:509:LEU:HD23	2.04	0.57
2:B:1211:THR:OG1	2:B:1233:TRP:HZ3	1.88	0.57
1:A:168:PRO:O	1:A:169:LEU:CD2	2.53	0.57
1:A:234:THR:HG23	1:A:274:GLY:O	2.05	0.57
2:B:742:ARG:HB3	2:B:742:ARG:HH11	1.70	0.57
2:B:811:LEU:HD23	2:B:905:LYS:HB2	1.86	0.57
1:A:84:VAL:HG13	1:A:101:VAL:HG21	1.87	0.56
1:A:363:TYR:CD1	1:A:364:ARG:CZ	2.87	0.56
1:A:580:VAL:HG21	2:B:747:GLU:HB3	1.87	0.56
1:A:590:THR:CB	1:A:593:LYS:HG3	2.31	0.56
2:B:744:GLU:CD	2:B:774:LYS:HD2	2.29	0.56
2:B:1028:LYS:HB2	2:B:1071:ILE:CG2	2.35	0.56
2:B:1341:LEU:HA	2:B:1367:CYS:O	2.05	0.56
2:B:799:PHE:HE1	2:B:801:VAL:HG23	1.69	0.56
1:A:127:ILE:HG22	1:A:128:PHE:N	2.20	0.56
1:A:430:SER:O	1:A:431:ASN:HB2	2.05	0.56
1:A:541:LEU:CD2	2:B:796:ALA:CB	2.80	0.56
1:A:566:ASP:CG	2:B:791:LYS:HG3	2.30	0.56
2:B:742:ARG:O	2:B:903:VAL:HG13	2.05	0.56
2:B:806:ASP:HB2	2:B:899:ILE:HD13	1.86	0.56
2:B:1259:GLN:HA	2:B:1259:GLN:OE1	2.01	0.56
2:B:1416:PHE:HZ	2:B:1442:HIS:CD2	2.20	0.56
1:A:61:MET:HE1	1:A:482:GLY:HA2	1.86	0.56
1:A:330:PRO:O	1:A:357:PRO:HG3	2.06	0.56
2:B:1387:THR:HG22	2:B:1451:GLN:N	2.21	0.56
1:A:327:VAL:CG2	1:A:357:PRO:CB	2.78	0.56
1:A:379:THR:HG22	1:A:380:GLN:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HD3	1:A:407:GLN:O	2.06	0.56
1:A:443:LEU:HB2	1:A:533:VAL:HG22	1.86	0.56
1:A:640:CYS:HB3	1:A:641:PRO:HD2	1.88	0.56
2:B:991:GLN:HE22	2:B:1104:HIS:HE1	1.50	0.56
2:B:1192:ALA:HB3	2:B:1195:LYS:HA	1.87	0.56
1:A:180:GLY:O	1:A:201:GLU:HG3	2.04	0.56
1:A:349:ASP:HB3	1:A:351:MET:CE	2.35	0.56
1:A:582:VAL:HG12	1:A:582:VAL:O	2.05	0.56
1:A:603:ILE:HG13	1:A:621:GLY:HA3	1.88	0.56
2:B:1392:ASP:C	2:B:1394:ASP:H	2.14	0.56
1:A:590:THR:HG22	1:A:592:SER:CB	2.35	0.56
2:B:1074:ASP:C	2:B:1076:GLN:H	2.13	0.56
2:B:1215:LEU:HA	2:B:1218:LEU:HD12	1.87	0.56
1:A:311:HIS:CE1	2:B:1410:TYR:HB3	2.41	0.56
1:A:408:GLU:C	1:A:409:LEU:HD12	2.31	0.56
2:B:829:LEU:CD2	2:B:840:VAL:HG11	2.35	0.56
2:B:932:ARG:O	2:B:932:ARG:HG3	2.04	0.56
2:B:978:LEU:CD2	2:B:981:LEU:HG	2.21	0.56
1:A:554:VAL:CG1	1:A:555:PRO:HD2	2.28	0.56
2:B:833:ARG:CG	2:B:833:ARG:NH1	2.67	0.56
1:A:365:VAL:O	1:A:365:VAL:HG13	2.06	0.56
2:B:741:SER:OG	2:B:891:LYS:HE2	2.06	0.56
1:A:343:LYS:HE2	1:A:527:ASP:OD1	2.06	0.55
2:B:1222:LYS:HA	2:B:1224:PHE:CZ	2.42	0.55
1:A:1:SER:N	1:A:2:PRO:HD3	2.21	0.55
2:B:744:GLU:HA	2:B:744:GLU:OE2	2.06	0.55
2:B:850:PHE:HZ	2:B:886:GLN:CB	2.19	0.55
2:B:1172:TYR:CD1	2:B:1216:LEU:HB3	2.40	0.55
1:A:19:THR:HG22	1:A:20:MET:N	2.21	0.55
1:A:441:THR:O	1:A:443:LEU:N	2.39	0.55
1:A:468:TYR:OH	1:A:486:ARG:HD2	2.06	0.55
1:A:591:GLN:CA	1:A:594:ILE:HG12	2.36	0.55
2:B:991:GLN:NE2	2:B:1104:HIS:CE1	2.74	0.55
2:B:799:PHE:HD1	2:B:800:GLU:N	1.92	0.55
2:B:811:LEU:O	2:B:905:LYS:HD2	2.06	0.55
2:B:1083:LYS:HE3	2:B:1141:ASN:OD1	2.05	0.55
2:B:1227:VAL:H	2:B:1228:PRO:HD2	1.71	0.55
2:B:1406:TYR:OH	2:B:1408:SER:HA	2.06	0.55
1:A:480:LYS:HZ1	1:A:497:LEU:HD13	1.70	0.55
1:A:598:VAL:HG12	1:A:598:VAL:O	2.05	0.55
2:B:833:ARG:HG2	2:B:833:ARG:NH1	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1343:VAL:HG11	2:B:1471:TYR:CD2	2.41	0.55
2:B:1128:SER:CA	2:B:1131:GLU:OE2	2.47	0.55
1:A:126:ARG:C	1:A:127:ILE:HD12	2.32	0.55
1:A:430:SER:O	1:A:431:ASN:OD1	2.23	0.55
2:B:999:THR:HG21	2:B:1026:LEU:O	2.07	0.55
2:B:1192:ALA:HA	2:B:1197:ARG:O	2.07	0.55
2:B:744:GLU:HG3	2:B:774:LYS:HB3	1.88	0.54
1:A:236:ARG:O	1:A:236:ARG:HG3	2.06	0.54
2:B:1296:LEU:HD23	2:B:1298:ARG:NH2	2.22	0.54
2:B:885:LEU:HD13	2:B:908:LYS:HG2	1.90	0.54
2:B:972:ALA:HB2	2:B:1261:GLN:HE21	1.72	0.54
1:A:364:ARG:H	1:A:379:THR:CG2	2.21	0.54
1:A:453:PHE:CD2	1:A:453:PHE:N	2.76	0.54
2:B:1145:GLY:O	2:B:1149:LYS:HG2	2.07	0.54
1:A:614:ALA:HA	1:A:632:THR:HG22	1.90	0.54
2:B:974:ASP:C	2:B:976:GLU:H	2.15	0.54
2:B:1370:TYR:HB2	2:B:1429:VAL:HG23	1.89	0.54
1:A:127:ILE:CG2	1:A:128:PHE:N	2.70	0.54
1:A:220:PHE:HB3	1:A:357:PRO:HG2	1.90	0.54
1:A:349:ASP:HB3	1:A:351:MET:HE3	1.89	0.54
2:B:744:GLU:HB2	2:B:775:ASP:CB	2.38	0.54
2:B:1363:ILE:HG12	2:B:1440:LYS:HG2	1.89	0.54
1:A:380:GLN:HE22	1:A:440:ARG:CZ	2.17	0.54
2:B:958:ILE:HG23	2:B:1322:VAL:HG22	1.90	0.54
2:B:1094:GLY:HA3	2:B:1150:ALA:HA	1.89	0.54
2:B:882:LYS:HG3	2:B:886:GLN:NE2	2.22	0.54
1:A:107:TYR:HB2	1:A:109:PHE:CE2	2.42	0.54
1:A:515:LEU:C	1:A:515:LEU:CD2	2.65	0.54
2:B:742:ARG:HB3	2:B:742:ARG:NH1	2.23	0.54
2:B:1028:LYS:HB2	2:B:1071:ILE:HG21	1.90	0.54
1:A:211:GLU:OE2	1:A:236:ARG:HD2	2.08	0.53
1:A:342:PHE:CD1	1:A:391:THR:HG21	2.43	0.53
2:B:1338:LYS:HA	2:B:1371:ARG:HD2	1.89	0.53
2:B:1094:GLY:HA3	2:B:1150:ALA:N	2.24	0.53
1:A:230:GLU:HG2	1:A:279:VAL:HG13	1.89	0.53
2:B:749:TRP:CB	2:B:774:LYS:HE2	2.38	0.53
2:B:1411:GLU:HG2	2:B:1422:LEU:CD1	2.37	0.53
3:M:23:LEU:HD11	3:M:51:ALA:O	2.09	0.53
1:A:133:LYS:O	1:A:134:LEU:HB2	2.09	0.53
1:A:455:LEU:HD23	1:A:486:ARG:NH2	2.23	0.53
1:A:501:THR:C	1:A:538:VAL:HG22	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LEU:HA	1:A:564:GLU:O	2.09	0.53
2:B:1213:TYR:HA	2:B:1216:LEU:HD12	1.91	0.53
1:A:187:TYR:HB2	1:A:194:GLN:O	2.09	0.53
1:A:458:ASP:N	1:A:458:ASP:OD1	2.41	0.53
1:A:556:GLY:C	3:M:39:TYR:HB2	2.33	0.53
1:A:637:GLU:HG3	1:A:639:GLN:O	2.08	0.53
2:B:782:ILE:O	2:B:798:PRO:CG	2.55	0.53
1:A:8:THR:HG22	1:A:20:MET:HB2	1.88	0.53
1:A:589:LEU:HD11	1:A:594:ILE:CD1	2.30	0.53
2:B:758:GLU:H	2:B:758:GLU:CD	2.16	0.53
2:B:1054:THR:OG1	2:B:1089:LYS:HG3	2.08	0.53
1:A:107:TYR:HB2	1:A:109:PHE:HZ	1.69	0.53
1:A:207:LEU:HD21	1:A:580:VAL:HG22	1.90	0.53
2:B:1047:PHE:CE2	2:B:1103:ILE:HD12	2.44	0.53
2:B:1106:GLU:HA	2:B:1112:ARG:CZ	2.39	0.53
2:B:1217:ALA:O	2:B:1219:LEU:N	2.42	0.53
2:B:1269:GLU:C	2:B:1270:LEU:CG	2.66	0.53
1:A:127:ILE:HD12	1:A:127:ILE:N	2.22	0.53
1:A:250:ILE:HG22	1:A:305:SER:HB3	1.91	0.53
1:A:264:GLU:O	1:A:284:VAL:HG11	2.09	0.53
1:A:468:TYR:CZ	1:A:486:ARG:HD2	2.43	0.53
2:B:1038:ARG:C	2:B:1039:GLN:O	2.51	0.53
2:B:1041:SER:HG	2:B:1084:TRP:CD1	2.26	0.53
1:A:18:GLU:O	1:A:66:PHE:CE2	2.62	0.53
1:A:427:VAL:HG23	1:A:613:TYR:CE2	2.44	0.53
1:A:441:THR:O	1:A:443:LEU:HG	2.09	0.53
2:B:783:LEU:N	2:B:798:PRO:CG	2.72	0.53
2:B:840:VAL:HG12	2:B:841:ARG:N	2.24	0.53
2:B:978:LEU:HB2	2:B:1240:TYR:HD1	1.74	0.53
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.09	0.53
2:B:1279:PRO:HB2	2:B:1306:GLU:CD	2.34	0.53
2:B:1095:VAL:HG13	2:B:1122:THR:OG1	2.09	0.52
2:B:1384:SER:HB2	2:B:1421:THR:HG22	1.92	0.52
2:B:1078:LEU:CD2	2:B:1135:ILE:HD13	2.39	0.52
2:B:1087:LEU:HD21	2:B:1142:SER:CB	2.39	0.52
2:B:1143:LEU:HD11	2:B:1147:ILE:HG13	1.91	0.52
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.44	0.52
2:B:1183:PRO:HG2	2:B:1184:LEU:HD12	1.91	0.52
1:A:345:GLY:C	1:A:346:MET:HG2	2.33	0.52
1:A:528:SER:CB	1:A:616:VAL:HG13	2.38	0.52
1:A:145:ILE:O	1:A:153:VAL:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLN:C	1:A:382:ASP:N	2.66	0.52
1:A:590:THR:HG22	1:A:592:SER:CA	2.39	0.52
2:B:733:ILE:HG13	2:B:894:VAL:O	2.09	0.52
2:B:729:LEU:HD13	2:B:729:LEU:C	2.34	0.52
2:B:1219:LEU:C	2:B:1221:LEU:H	2.17	0.52
1:A:78:LYS:HE3	1:A:82:LYS:NZ	2.25	0.52
1:A:113:ASP:OD2	2:B:748:SER:CB	2.57	0.52
2:B:744:GLU:CB	2:B:775:ASP:N	2.72	0.52
1:A:208:PRO:HD2	1:A:583:LEU:HD11	1.92	0.52
1:A:327:VAL:HG21	1:A:357:PRO:HG3	1.92	0.52
1:A:380:GLN:NE2	1:A:440:ARG:NH1	2.25	0.52
1:A:541:LEU:HG	2:B:796:ALA:HB1	1.77	0.52
2:B:865:THR:O	2:B:865:THR:HG22	2.08	0.52
1:A:164:LEU:HD23	1:A:570:ARG:HB2	1.92	0.52
3:M:73:ILE:O	3:M:73:ILE:HG13	2.09	0.52
1:A:364:ARG:N	1:A:379:THR:CG2	2.73	0.52
1:A:504:ILE:HG23	1:A:535:ASP:HA	1.92	0.52
2:B:1037:PHE:HA	2:B:1048:VAL:CG1	2.40	0.52
2:B:1102:VAL:O	2:B:1105:GLN:HG2	2.09	0.52
3:M:47:SER:O	3:M:70:LEU:HD13	2.10	0.52
1:A:380:GLN:HG3	1:A:384:VAL:O	2.09	0.52
2:B:749:TRP:CZ3	2:B:750:LEU:HB2	2.45	0.52
2:B:1062:LYS:HE3	2:B:1124:PHE:CZ	2.45	0.52
1:A:591:GLN:OE1	1:A:594:ILE:HG13	2.10	0.51
2:B:916:MET:O	2:B:1325:MET:HG3	2.09	0.51
2:B:1086:ILE:HG21	2:B:1142:SER:HB2	1.91	0.51
1:A:141:VAL:HG12	1:A:142:MET:N	2.25	0.51
2:B:756:LEU:HD22	2:B:765:SER:HB2	1.91	0.51
2:B:777:ILE:HD12	2:B:808:PHE:CB	2.39	0.51
2:B:819:ARG:HG2	2:B:820:ASN:ND2	2.26	0.51
2:B:1260:TYR:CG	2:B:1260:TYR:O	2.63	0.51
2:B:1366:ILE:HG21	2:B:1455:VAL:HG11	1.92	0.51
1:A:613:TYR:O	1:A:617:PHE:CD2	2.64	0.51
2:B:1158:TYR:OH	2:B:1188:PHE:HB2	2.11	0.51
1:A:37:VAL:O	1:A:46:VAL:HG22	2.10	0.51
1:A:386:LYS:HZ3	1:A:440:ARG:HG2	1.75	0.51
2:B:1038:ARG:HD3	2:B:1077:VAL:CG1	2.40	0.51
1:A:541:LEU:CB	2:B:796:ALA:HB2	2.37	0.51
1:A:591:GLN:HB2	2:B:795:VAL:HB	1.90	0.51
1:A:366:PRO:HA	1:A:377:SER:O	2.11	0.51
1:A:439:LEU:CD1	1:A:450:ASN:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:SER:O	1:A:238:LEU:HG	2.10	0.51
1:A:209:SER:C	1:A:238:LEU:HG	2.36	0.51
1:A:365:VAL:N	1:A:379:THR:OG1	2.20	0.51
1:A:432:ASN:HB2	1:A:523:GLU:OE1	2.10	0.51
1:A:511:ALA:O	1:A:512:TYR:HB3	2.11	0.51
1:A:530:TRP:CD2	1:A:607:PRO:CB	2.94	0.51
1:A:561:LEU:O	1:A:563:ILE:HD12	2.11	0.51
1:A:617:PHE:HB2	1:A:632:THR:HG21	1.92	0.51
2:B:734:ILE:HD11	2:B:898:PHE:HD2	1.76	0.51
1:A:114:LYS:HB2	1:A:117:TYR:CZ	2.46	0.50
1:A:428:GLY:C	1:A:430:SER:N	2.68	0.50
2:B:1113:ASN:C	2:B:1115:ASN:H	2.17	0.50
1:A:179:MET:CG	1:A:203:LYS:HA	2.41	0.50
1:A:516:ILE:CG1	1:A:522:ARG:HD2	2.40	0.50
1:A:187:TYR:CD1	1:A:192:PRO:HA	2.46	0.50
2:B:842:VAL:HG22	2:B:876:TYR:OH	2.11	0.50
2:B:1255:GLN:HA	2:B:1258:ALA:HB3	1.93	0.50
2:B:1277:GLN:HG3	2:B:1281:ARG:NE	2.26	0.50
1:A:147:ASN:HB3	1:A:182:TRP:CZ3	2.46	0.50
1:A:509:LEU:HD13	1:A:509:LEU:O	2.09	0.50
2:B:903:VAL:HG11	2:B:905:LYS:HE3	1.92	0.50
2:B:1026:LEU:HD23	2:B:1029:LYS:HD3	1.93	0.50
2:B:1071:ILE:HD11	2:B:1073:ILE:HD11	1.93	0.50
2:B:1107:MET:O	2:B:1248:GLN:HG2	2.10	0.50
2:B:1260:TYR:O	2:B:1260:TYR:CD2	2.65	0.50
2:B:1397:LYS:HZ1	2:B:1412:LEU:HG	1.71	0.50
1:A:239:TYR:HA	2:B:779:THR:OG1	2.11	0.50
1:A:437:SER:OG	1:A:452:ASN:HB2	2.12	0.50
1:A:517:GLY:O	1:A:518:ALA:CB	2.60	0.50
2:B:799:PHE:C	2:B:800:GLU:HG3	2.33	0.50
2:B:1064:PHE:O	2:B:1068:VAL:HG13	2.11	0.50
1:A:141:VAL:C	1:A:142:MET:SD	2.94	0.50
2:B:1035:LEU:HD21	2:B:1077:VAL:HG21	1.94	0.50
2:B:1457:VAL:HG22	2:B:1467:CYS:O	2.12	0.50
1:A:220:PHE:CZ	1:A:330:PRO:CB	2.89	0.50
1:A:221:TYR:HE1	1:A:228:GLY:CA	2.23	0.50
1:A:507:PHE:HE1	1:A:533:VAL:CG2	2.25	0.50
1:A:20:MET:SD	1:A:20:MET:C	2.95	0.50
1:A:109:PHE:HD2	1:A:128:PHE:O	1.95	0.50
1:A:110:ILE:HG22	1:A:111:GLN:N	2.26	0.50
1:A:163:GLN:HG2	1:A:167:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLN:O	1:A:194:GLN:OE1	2.30	0.50
2:B:1259:GLN:OE1	2:B:1262:LYS:HD3	2.12	0.50
2:B:1408:SER:C	2:B:1410:TYR:H	2.20	0.50
1:A:154:LYS:HG2	1:A:155:GLN:N	2.26	0.50
2:B:930:LEU:HD12	2:B:936:GLN:HE22	1.76	0.50
2:B:1053:SER:OG	2:B:1102:VAL:HG13	2.12	0.50
2:B:1211:THR:OG1	2:B:1233:TRP:CZ3	2.64	0.50
2:B:1276:LEU:O	2:B:1285:ILE:HD12	2.12	0.50
3:M:20:LYS:HD3	3:M:55:LEU:HD21	1.93	0.50
1:A:331:TYR:O	1:A:415:ALA:CB	2.60	0.49
1:A:365:VAL:H	1:A:379:THR:HG1	1.52	0.49
2:B:791:LYS:O	2:B:792:GLY:C	2.54	0.49
2:B:964:PRO:HB3	2:B:1270:LEU:CG	2.41	0.49
2:B:1219:LEU:C	2:B:1221:LEU:N	2.70	0.49
1:A:36:THR:HA	1:A:48:SER:HA	1.94	0.49
1:A:207:LEU:CD2	2:B:747:GLU:HG2	2.34	0.49
1:A:409:LEU:HB2	1:A:414:GLN:OE1	2.12	0.49
1:A:427:VAL:HG22	1:A:613:TYR:CE2	2.47	0.49
1:A:590:THR:CG2	1:A:592:SER:CB	2.90	0.49
2:B:1038:ARG:HD3	2:B:1077:VAL:HG13	1.94	0.49
2:B:1269:GLU:O	2:B:1269:GLU:OE1	2.30	0.49
2:B:1315:LYS:H	2:B:1315:LYS:HD2	1.76	0.49
2:B:1340:ASP:O	2:B:1368:THR:HA	2.12	0.49
1:A:580:VAL:HG21	2:B:747:GLU:CB	2.41	0.49
2:B:1341:LEU:HD12	2:B:1367:CYS:O	2.11	0.49
2:B:1399:LEU:HB3	2:B:1405:ARG:NH1	2.28	0.49
1:A:13:ARG:HD2	1:A:18:GLU:OE2	2.11	0.49
2:B:1036:ALA:O	2:B:1037:PHE:CG	2.66	0.49
2:B:1120:ALA:HA	2:B:1169:ILE:HD13	1.92	0.49
2:B:1126:LEU:CD2	2:B:1173:ALA:HB1	2.35	0.49
1:A:369:VAL:H	1:A:375:VAL:CG1	2.26	0.49
1:A:516:ILE:CD1	1:A:522:ARG:HD3	2.34	0.49
1:A:605:CYS:C	1:A:607:PRO:HD3	2.37	0.49
2:B:843:GLU:HG2	2:B:845:LEU:HD12	1.93	0.49
2:B:885:LEU:CD1	2:B:908:LYS:HG2	2.42	0.49
1:A:37:VAL:HG13	1:A:86:VAL:HG22	1.94	0.49
1:A:453:PHE:O	1:A:492:LEU:HA	2.13	0.49
1:A:522:ARG:HH11	1:A:522:ARG:HG2	1.71	0.49
2:B:811:LEU:HD13	2:B:890:VAL:HG22	1.94	0.49
2:B:838:LEU:HB3	2:B:894:VAL:HG11	1.94	0.49
2:B:1000:VAL:HG22	2:B:1027:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1078:LEU:HD21	2:B:1135:ILE:HD13	1.94	0.49
2:B:1113:ASN:C	2:B:1115:ASN:N	2.71	0.49
2:B:1288:ARG:HD3	2:B:1290:HIS:NE2	2.27	0.49
2:B:1399:LEU:HB3	2:B:1405:ARG:HH11	1.77	0.49
3:M:26:LEU:HD13	3:M:70:LEU:HD11	1.94	0.49
1:A:147:ASN:HB3	1:A:182:TRP:CH2	2.48	0.49
1:A:253:ILE:O	1:A:260:ILE:HG12	2.12	0.49
1:A:559:MET:O	1:A:559:MET:HG3	2.12	0.49
2:B:1078:LEU:HD11	2:B:1132:ALA:HB1	1.94	0.49
2:B:1259:GLN:HE22	2:B:1262:LYS:CG	2.26	0.49
2:B:1403:VAL:HG22	2:B:1404:ASP:N	2.27	0.49
1:A:168:PRO:O	1:A:169:LEU:HG	2.13	0.49
1:A:404:THR:CG2	1:A:414:GLN:HB3	2.41	0.49
2:B:744:GLU:HB2	2:B:775:ASP:CA	2.42	0.49
2:B:1004:HIS:HB2	2:B:1066:LEU:HD21	1.95	0.49
3:M:65:GLU:HG3	3:M:65:GLU:O	2.12	0.49
1:A:22:LEU:HD13	1:A:52:THR:HG21	1.94	0.49
1:A:350:LEU:C	1:A:351:MET:HE2	2.38	0.49
1:A:557:GLN:HG2	1:A:558:GLN:N	2.28	0.49
2:B:742:ARG:HD2	2:B:775:ASP:O	2.13	0.49
2:B:1094:GLY:HA3	2:B:1150:ALA:CA	2.42	0.49
1:A:10:ASN:OD1	1:A:618:SER:HA	2.12	0.49
2:B:782:ILE:HB	2:B:798:PRO:HB2	1.92	0.49
2:B:866:ILE:HG12	2:B:872:LEU:HD22	1.95	0.49
2:B:964:PRO:HB3	2:B:1270:LEU:CD2	2.43	0.49
2:B:974:ASP:HB3	2:B:976:GLU:HG3	1.95	0.49
2:B:993:MET:HE1	2:B:1063:VAL:HB	1.93	0.49
2:B:1184:LEU:HD12	2:B:1184:LEU:N	2.28	0.49
2:B:1290:HIS:O	2:B:1294:ALA:HB2	2.13	0.49
2:B:1347:PRO:HG3	2:B:1362:MET:HE2	1.94	0.49
1:A:140:THR:C	1:A:141:VAL:CG2	2.86	0.48
1:A:501:THR:O	1:A:504:ILE:HD12	2.13	0.48
2:B:734:ILE:HG12	3:M:46:ILE:HG23	1.95	0.48
2:B:1025:GLU:O	2:B:1026:LEU:HD23	2.13	0.48
2:B:1172:TYR:CE2	2:B:1216:LEU:HD13	2.48	0.48
2:B:1239:TYR:CD2	2:B:1253:VAL:HG11	2.47	0.48
1:A:352:VAL:O	1:A:384:VAL:HG22	2.13	0.48
2:B:733:ILE:HG12	2:B:734:ILE:N	2.21	0.48
1:A:6:ILE:HD11	1:A:20:MET:CG	2.41	0.48
1:A:221:TYR:HD2	1:A:326:ILE:HD12	1.78	0.48
1:A:268:ARG:NE	2:B:1406:TYR:CD2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:HD2	1:A:343:LYS:N	2.27	0.48
1:A:386:LYS:NZ	1:A:440:ARG:HG2	2.27	0.48
2:B:847:ASN:C	2:B:849:ALA:H	2.21	0.48
2:B:1113:ASN:HD22	2:B:1163:ARG:NE	2.11	0.48
2:B:1215:LEU:HD13	2:B:1230:VAL:CG1	2.43	0.48
2:B:733:ILE:C	2:B:734:ILE:HD12	2.38	0.48
1:A:137:VAL:CG2	1:A:139:ARG:NH1	2.76	0.48
2:B:804:MET:HG2	2:B:805:GLN:H	1.78	0.48
2:B:1203:LYS:HD2	2:B:1206:TYR:CE2	2.49	0.48
2:B:1409:LYS:O	2:B:1409:LYS:HG2	2.11	0.48
2:B:1457:VAL:HG23	2:B:1457:VAL:O	2.14	0.48
1:A:333:ILE:O	1:A:417:ARG:HG2	2.13	0.48
1:A:509:LEU:O	1:A:529:VAL:HG12	2.13	0.48
2:B:730:ASP:O	3:M:53:TYR:HD1	1.97	0.48
2:B:782:ILE:HG22	2:B:798:PRO:HB3	1.94	0.48
2:B:925:LEU:O	2:B:926:ASP:HB2	2.13	0.48
2:B:733:ILE:HD11	2:B:893:ALA:O	2.13	0.48
2:B:1253:VAL:O	2:B:1257:LEU:HD12	2.13	0.48
3:M:15:LEU:HG	3:M:63:MET:HB3	1.96	0.48
1:A:145:ILE:HG21	1:A:171:TRP:CE3	2.49	0.48
2:B:898:PHE:HB2	3:M:50:LYS:HE3	1.96	0.48
2:B:1475:LYS:HE2	2:B:1493:GLU:OE2	2.13	0.48
1:A:304:VAL:HG12	1:A:305:SER:N	2.28	0.48
1:A:501:THR:CB	1:A:538:VAL:HG13	2.43	0.48
2:B:841:ARG:HB2	2:B:895:TYR:CE1	2.48	0.48
2:B:1408:SER:C	2:B:1410:TYR:N	2.72	0.48
2:B:1175:ALA:HB1	2:B:1221:LEU:HD21	1.95	0.48
2:B:1392:ASP:O	2:B:1394:ASP:N	2.46	0.48
1:A:314:SER:OG	2:B:828:VAL:HG22	2.14	0.47
1:A:462:GLU:HB2	1:A:486:ARG:HH22	1.79	0.47
1:A:465:ILE:HD11	1:A:515:LEU:HB3	1.95	0.47
2:B:1012:TRP:CH2	2:B:1020:ARG:HB2	2.49	0.47
2:B:1172:TYR:CD2	2:B:1216:LEU:HD13	2.49	0.47
2:B:1219:LEU:HD23	2:B:1227:VAL:HG21	1.95	0.47
2:B:1477:ASP:OD2	2:B:1479:LYS:HD3	2.13	0.47
3:M:54:ALA:CB	3:M:62:LYS:HB3	2.44	0.47
1:A:12:LEU:O	1:A:13:ARG:HG3	2.14	0.47
1:A:509:LEU:HD22	1:A:510:VAL:H	1.79	0.47
1:A:571:VAL:HB	2:B:754:GLU:O	2.14	0.47
2:B:744:GLU:HB2	2:B:775:ASP:N	2.29	0.47
2:B:782:ILE:HD12	2:B:799:PHE:CD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1047:PHE:HE2	2:B:1103:ILE:HD12	1.78	0.47
2:B:1415:ALA:O	2:B:1419:ARG:NH1	2.47	0.47
3:M:71:GLN:HE21	3:M:71:GLN:HA	1.79	0.47
1:A:10:ASN:HB2	1:A:622:LEU:N	2.29	0.47
1:A:38:HIS:O	1:A:85:THR:HB	2.14	0.47
1:A:133:LYS:HG2	1:A:477:ARG:HD3	1.95	0.47
1:A:222:TYR:CD1	1:A:328:THR:HA	2.49	0.47
1:A:246:THR:HG21	2:B:1425:TYR:CE1	2.49	0.47
2:B:1039:GLN:HB3	2:B:1040:PRO:CD	2.44	0.47
3:M:26:LEU:O	3:M:26:LEU:HG	2.14	0.47
3:M:71:GLN:O	3:M:71:GLN:HG3	2.15	0.47
1:A:114:LYS:HE3	1:A:117:TYR:CE1	2.49	0.47
1:A:433:TYR:CD2	1:A:456:ARG:HG2	2.46	0.47
1:A:508:ARG:HH21	1:A:607:PRO:HG3	1.80	0.47
1:A:541:LEU:HD12	1:A:542:VAL:N	2.30	0.47
2:B:1034:GLN:C	2:B:1036:ALA:H	2.22	0.47
2:B:1055:TRP:HE3	2:B:1102:VAL:HG11	1.79	0.47
1:A:108:LEU:HB2	1:A:196:PHE:CE1	2.50	0.47
1:A:397:PRO:HB3	1:A:420:GLN:HE21	1.78	0.47
1:A:515:LEU:CD2	1:A:523:GLU:HB3	2.45	0.47
2:B:944:ASP:O	2:B:945:LEU:C	2.58	0.47
3:M:20:LYS:HD3	3:M:55:LEU:CD2	2.44	0.47
2:B:1475:LYS:HD2	2:B:1475:LYS:N	2.27	0.47
1:A:145:ILE:HG21	1:A:171:TRP:CZ3	2.50	0.47
1:A:188:TYR:HD1	1:A:194:GLN:HE22	1.62	0.47
1:A:239:TYR:HE1	2:B:832:TYR:CZ	2.33	0.47
1:A:400:ILE:O	1:A:418:THR:HA	2.14	0.47
1:A:469:THR:O	1:A:511:ALA:HA	2.15	0.47
2:B:744:GLU:HG3	2:B:774:LYS:CA	2.44	0.47
2:B:882:LYS:HG3	2:B:886:GLN:CD	2.40	0.47
2:B:920:VAL:CG2	2:B:1324:THR:HG23	2.45	0.47
2:B:991:GLN:OE1	2:B:1104:HIS:CE1	2.67	0.47
2:B:996:MET:HE1	2:B:1030:GLY:CA	2.41	0.47
2:B:1066:LEU:HD23	2:B:1066:LEU:O	2.14	0.47
2:B:1082:VAL:HG22	2:B:1129:LEU:HD22	1.97	0.47
3:M:43:THR:HG22	3:M:43:THR:O	2.14	0.47
3:M:54:ALA:HB1	3:M:62:LYS:HB3	1.97	0.47
1:A:31:VAL:HG11	1:A:54:LEU:HD12	1.97	0.47
1:A:363:TYR:HD2	1:A:381:GLY:HA2	1.80	0.47
1:A:439:LEU:HD13	1:A:450:ASN:HB2	1.96	0.47
2:B:736:GLU:OE2	2:B:845:LEU:HD21	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:749:TRP:CD2	2:B:774:LYS:HG2	2.50	0.47
2:B:1278:LEU:O	2:B:1281:ARG:CD	2.62	0.47
1:A:1:SER:H3	1:A:2:PRO:HD3	1.79	0.47
1:A:262:LEU:CD2	1:A:288:GLY:HA3	2.45	0.47
2:B:1407:ILE:O	2:B:1408:SER:C	2.57	0.47
1:A:58:THR:O	1:A:61:MET:HB2	2.14	0.47
1:A:168:PRO:O	1:A:169:LEU:CG	2.63	0.47
1:A:370:GLN:HB2	1:A:401:THR:O	2.15	0.47
1:A:468:TYR:CE2	1:A:486:ARG:HD2	2.49	0.47
1:A:512:TYR:HB2	1:A:525:VAL:O	2.15	0.47
2:B:756:LEU:HD22	2:B:765:SER:CB	2.45	0.47
2:B:817:VAL:CG2	2:B:907:LEU:HD11	2.45	0.47
2:B:927:PRO:HG2	2:B:1313:GLU:CA	2.44	0.47
1:A:55:THR:C	1:A:57:ALA:H	2.24	0.46
1:A:109:PHE:HE2	1:A:130:VAL:CG2	2.27	0.46
1:A:136:PRO:HG3	2:B:789:ASP:HA	1.97	0.46
1:A:147:ASN:HB2	1:A:148:PRO:HD3	1.96	0.46
1:A:268:ARG:HD2	2:B:1425:TYR:CD1	2.50	0.46
2:B:734:ILE:CD1	2:B:898:PHE:HD2	2.27	0.46
2:B:811:LEU:HD22	2:B:903:VAL:O	2.14	0.46
2:B:1163:ARG:C	2:B:1165:TYR:H	2.23	0.46
2:B:1281:ARG:O	2:B:1281:ARG:CG	2.63	0.46
3:M:14:LYS:O	3:M:14:LYS:HG2	2.15	0.46
1:A:176:LEU:HD21	2:B:1327:HIS:NE2	2.30	0.46
2:B:1410:TYR:O	2:B:1410:TYR:CD2	2.68	0.46
1:A:187:TYR:CG	1:A:195:VAL:HG22	2.50	0.46
1:A:207:LEU:HG	1:A:579:GLY:O	2.15	0.46
1:A:269:ILE:HD12	1:A:277:GLU:O	2.15	0.46
1:A:555:PRO:HB3	2:B:775:ASP:CA	2.39	0.46
2:B:889:GLU:OE2	2:B:891:LYS:CE	2.64	0.46
2:B:1276:LEU:C	2:B:1285:ILE:HD12	2.40	0.46
1:A:475:LYS:HD2	1:A:598:VAL:HG11	1.98	0.46
2:B:889:GLU:OE2	2:B:891:LYS:HE3	2.16	0.46
2:B:1091:LYS:HB3	2:B:1092:PRO:CD	2.45	0.46
1:A:113:ASP:OD2	2:B:748:SER:HB3	2.14	0.46
1:A:22:LEU:HD13	1:A:52:THR:CG2	2.46	0.46
1:A:35:VAL:CG1	1:A:36:THR:N	2.79	0.46
1:A:100:LEU:HD22	1:A:636:ALA:C	2.40	0.46
1:A:139:ARG:O	1:A:159:SER:OG	2.29	0.46
2:B:733:ILE:HG23	2:B:734:ILE:N	2.29	0.46
1:A:541:LEU:CD2	2:B:786:SER:HB3	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:VAL:CB	2:B:751:TRP:CE3	2.98	0.46
1:A:61:MET:HE3	1:A:61:MET:HB3	1.55	0.46
1:A:238:LEU:HD22	1:A:578:LYS:HB3	1.98	0.46
1:A:339:PRO:HG3	1:A:608:GLY:HA2	1.98	0.46
1:A:394:SER:C	1:A:396:LYS:H	2.22	0.46
3:M:6:THR:H	3:M:9:GLU:HB3	1.81	0.46
2:B:838:LEU:HB3	2:B:894:VAL:CG1	2.46	0.46
2:B:1275:SER:OG	2:B:1311:THR:HB	2.16	0.46
3:M:72:LYS:O	3:M:76:GLU:HG3	2.16	0.46
1:A:36:THR:HG22	1:A:37:VAL:N	2.31	0.46
1:A:356:ASN:HB3	1:A:357:PRO:CD	2.46	0.46
1:A:451:VAL:HG23	1:A:495:LEU:O	2.16	0.46
1:A:553:PRO:O	2:B:803:VAL:HG13	2.16	0.46
2:B:1219:LEU:HD21	2:B:1227:VAL:HG21	1.97	0.46
2:B:1429:VAL:HG23	2:B:1429:VAL:O	2.15	0.46
2:B:1457:VAL:O	2:B:1466:SER:HA	2.16	0.46
3:M:53:TYR:O	3:M:56:LYS:HG3	2.16	0.46
1:A:363:TYR:HD1	1:A:364:ARG:CZ	2.30	0.45
2:B:754:GLU:HG3	2:B:769:MET:SD	2.56	0.45
2:B:807:PHE:HB3	2:B:899:ILE:HG21	1.97	0.45
2:B:876:TYR:HA	2:B:1451:GLN:NE2	2.30	0.45
2:B:949:VAL:HG23	2:B:1328:ALA:O	2.16	0.45
2:B:1296:LEU:HD23	2:B:1298:ARG:HH22	1.81	0.45
2:B:1325:MET:HE3	2:B:1325:MET:HB2	1.85	0.45
1:A:173:ILE:HD13	1:A:202:VAL:CG2	2.47	0.45
1:A:268:ARG:CZ	1:A:268:ARG:HB3	2.44	0.45
1:A:335:PHE:HE2	1:A:417:ARG:HG3	1.78	0.45
1:A:428:GLY:O	1:A:429:ASN:HB3	2.16	0.45
1:A:530:TRP:HB2	1:A:607:PRO:HB3	1.98	0.45
2:B:957:ARG:O	2:B:1322:VAL:HG13	2.17	0.45
1:A:131:ASN:HD21	1:A:133:LYS:CD	2.24	0.45
2:B:1029:LYS:O	2:B:1033:GLN:HG3	2.16	0.45
3:M:50:LYS:HE2	3:M:65:GLU:CG	2.45	0.45
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.51	0.45
1:A:316:MET:HE3	1:A:318:GLN:HE21	1.80	0.45
1:A:484:GLN:HG3	1:A:485:VAL:N	2.30	0.45
1:A:560:THR:HA	2:B:769:MET:O	2.17	0.45
2:B:1033:GLN:O	2:B:1036:ALA:HB3	2.16	0.45
2:B:1237:GLN:O	2:B:1238:ARG:C	2.60	0.45
2:B:1289:ILE:HG23	2:B:1294:ALA:HA	1.97	0.45
3:M:19:LEU:HG	3:M:19:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:C	1:A:51:LYS:HG2	2.41	0.45
1:A:115:THR:HG23	1:A:581:PHE:HE1	1.82	0.45
1:A:116:ILE:HG13	1:A:201:GLU:O	2.16	0.45
1:A:284:VAL:HG12	1:A:284:VAL:O	2.15	0.45
1:A:339:PRO:HG3	1:A:608:GLY:CA	2.47	0.45
1:A:397:PRO:CB	1:A:420:GLN:HE21	2.29	0.45
2:B:778:THR:OG1	2:B:779:THR:N	2.50	0.45
2:B:981:LEU:HD13	2:B:1002:ALA:HB2	1.97	0.45
2:B:1227:VAL:H	2:B:1228:PRO:CD	2.29	0.45
2:B:1260:TYR:C	2:B:1263:ASP:OD1	2.59	0.45
2:B:1369:ARG:HG3	2:B:1433:GLU:O	2.15	0.45
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.51	0.45
3:M:15:LEU:HD21	3:M:64:SER:HB2	1.98	0.45
1:A:239:TYR:HE1	2:B:832:TYR:CE1	2.34	0.45
1:A:451:VAL:O	1:A:453:PHE:CE2	2.70	0.45
1:A:497:LEU:HD12	1:A:498:SER:H	1.82	0.45
2:B:730:ASP:O	3:M:53:TYR:CD1	2.70	0.45
2:B:1387:THR:CG2	2:B:1450:ILE:HA	2.47	0.45
2:B:1431:HIS:H	2:B:1431:HIS:CD2	2.34	0.45
1:A:11:ILE:HG12	1:A:100:LEU:HD23	1.98	0.45
1:A:47:LEU:C	1:A:47:LEU:HD23	2.41	0.45
1:A:63:ASN:HD22	4:A:646:NAG:H83	1.81	0.45
1:A:109:PHE:O	1:A:127:ILE:HA	2.17	0.45
1:A:267:LYS:O	2:B:1378:MET:HE1	2.17	0.45
2:B:954:SER:HB3	2:B:1326:TYR:CB	2.47	0.45
2:B:1230:VAL:O	2:B:1230:VAL:HG12	2.17	0.45
1:A:248:PHE:CZ	2:B:1380:ILE:HG12	2.52	0.45
1:A:507:PHE:CE1	1:A:533:VAL:HG23	2.51	0.45
2:B:1221:LEU:O	2:B:1222:LYS:CB	2.65	0.45
2:B:1281:ARG:O	2:B:1281:ARG:HG2	2.17	0.45
1:A:117:TYR:HD2	1:A:200:PHE:CD1	2.34	0.45
4:A:646:NAG:O4	4:A:647:NAG:C1	2.65	0.45
2:B:756:LEU:CD1	2:B:765:SER:HB2	2.39	0.45
2:B:782:ILE:CG2	2:B:798:PRO:HB3	2.47	0.45
2:B:956:THR:CG2	2:B:1324:THR:HG22	2.47	0.45
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.81	0.45
1:A:516:ILE:O	1:A:516:ILE:HG23	2.16	0.45
1:A:615:GLY:O	1:A:619:ASP:CG	2.60	0.45
1:A:641:PRO:O	1:A:642:GLN:C	2.60	0.45
2:B:954:SER:CB	2:B:1326:TYR:HB3	2.45	0.45
2:B:1023:ALA:C	2:B:1025:GLU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1239:TYR:HD2	2:B:1253:VAL:HG11	1.81	0.45
1:A:370:GLN:NE2	1:A:403:ARG:NE	2.56	0.44
1:A:400:ILE:O	1:A:418:THR:HG23	2.17	0.44
1:A:140:THR:C	1:A:141:VAL:HG23	2.43	0.44
1:A:233:ILE:CG2	1:A:271:ILE:HD11	2.48	0.44
1:A:346:MET:HE1	1:A:454:LEU:HG	1.98	0.44
1:A:508:ARG:NH2	1:A:604:GLY:C	2.75	0.44
2:B:918:LYS:HE3	2:B:1326:TYR:OH	2.17	0.44
2:B:964:PRO:CB	2:B:1270:LEU:HD21	2.45	0.44
2:B:1091:LYS:HB3	2:B:1092:PRO:HD2	2.00	0.44
2:B:1191:THR:HG22	2:B:1198:TRP:CD1	2.52	0.44
2:B:1232:ARG:O	2:B:1232:ARG:HG2	2.17	0.44
3:M:67:LYS:HB3	3:M:67:LYS:HE2	1.66	0.44
1:A:179:MET:HE3	1:A:204:GLU:HG3	1.99	0.44
1:A:430:SER:C	1:A:431:ASN:CG	2.82	0.44
1:A:591:GLN:HA	1:A:591:GLN:OE1	2.17	0.44
2:B:1193:LYS:C	2:B:1195:LYS:H	2.25	0.44
2:B:1476:GLU:HG3	2:B:1477:ASP:N	2.32	0.44
1:A:516:ILE:CG1	1:A:522:ARG:CD	2.95	0.44
1:A:573:LEU:HG	2:B:752:ASN:O	2.17	0.44
2:B:805:GLN:HG2	2:B:806:ASP:N	2.30	0.44
2:B:1117:LYS:O	2:B:1118:ASP:OD1	2.35	0.44
2:B:1140:VAL:O	2:B:1140:VAL:HG12	2.16	0.44
2:B:1269:GLU:O	2:B:1270:LEU:CD2	2.57	0.44
1:A:265:SER:O	1:A:267:LYS:HG2	2.18	0.44
2:B:964:PRO:CB	2:B:1291:TRP:CZ3	3.01	0.44
2:B:967:GLN:HB3	2:B:968:MET:H	1.69	0.44
2:B:1126:LEU:HD11	2:B:1177:MET:HE1	1.99	0.44
2:B:1128:SER:C	2:B:1129:LEU:HD23	2.42	0.44
2:B:1143:LEU:CD1	2:B:1147:ILE:HG13	2.48	0.44
2:B:1262:LYS:HE2	2:B:1262:LYS:HB2	1.73	0.44
1:A:3:MET:HG2	1:A:4:TYR:N	2.33	0.44
1:A:179:MET:CE	1:A:204:GLU:HG3	2.47	0.44
1:A:309:ILE:HD11	1:A:316:MET:SD	2.58	0.44
2:B:759:PRO:HA	2:B:760:PRO:HD3	1.87	0.44
1:A:34:THR:HG22	1:A:51:LYS:HE3	2.00	0.44
1:A:55:THR:CB	1:A:57:ALA:H	2.29	0.44
2:B:744:GLU:CG	2:B:774:LYS:HB3	2.47	0.44
2:B:754:GLU:HB3	2:B:767:LYS:HE3	1.99	0.44
2:B:959:LEU:HD21	2:B:961:GLN:HB2	2.00	0.44
2:B:1213:TYR:HD1	2:B:1216:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:HA	1:A:623:THR:HG23	1.99	0.44
1:A:132:HIS:C	1:A:133:LYS:CG	2.90	0.44
1:A:333:ILE:HD12	1:A:416:THR:HA	2.00	0.44
2:B:940:ILE:HD12	2:B:1308:PHE:CZ	2.52	0.44
2:B:948:GLN:NE2	2:B:954:SER:HB3	2.33	0.44
2:B:1063:VAL:O	2:B:1063:VAL:HG12	2.17	0.44
2:B:1120:ALA:HA	2:B:1169:ILE:HG21	1.99	0.44
2:B:1448:GLU:O	2:B:1448:GLU:HG3	2.18	0.44
1:A:149:GLU:CD	1:A:178:ASN:HD22	2.26	0.44
1:A:565:GLY:O	2:B:764:ILE:HA	2.17	0.44
2:B:998:PRO:HA	2:B:1001:ILE:HG22	2.00	0.44
2:B:1107:MET:HE3	2:B:1247:THR:HG21	2.00	0.44
3:M:18:GLU:O	3:M:67:LYS:HG3	2.18	0.44
1:A:451:VAL:O	1:A:453:PHE:HE2	2.01	0.43
1:A:530:TRP:CG	1:A:607:PRO:CB	2.99	0.43
2:B:954:SER:CB	2:B:1326:TYR:CB	2.95	0.43
2:B:1203:LYS:HB2	2:B:1206:TYR:CD2	2.53	0.43
3:M:44:ILE:HD11	3:M:74:TYR:HE1	1.82	0.43
1:A:346:MET:SD	1:A:435:HIS:HB2	2.59	0.43
2:B:998:PRO:C	2:B:1001:ILE:HG22	2.43	0.43
2:B:1086:ILE:CD1	2:B:1143:LEU:HA	2.48	0.43
2:B:1267:HIS:O	2:B:1267:HIS:CG	2.70	0.43
2:B:1310:VAL:HG12	2:B:1311:THR:N	2.33	0.43
1:A:7:ILE:CG2	1:A:8:THR:H	2.29	0.43
1:A:19:THR:O	1:A:20:MET:CB	2.65	0.43
1:A:343:LYS:HE2	1:A:527:ASP:CG	2.43	0.43
1:A:361:PRO:CB	1:A:382:ASP:O	2.66	0.43
2:B:1162:GLN:O	2:B:1163:ARG:C	2.62	0.43
2:B:1462:ASN:HD22	2:B:1462:ASN:HA	1.59	0.43
1:A:62:GLY:C	1:A:63:ASN:CG	2.86	0.43
1:A:516:ILE:HD12	1:A:522:ARG:CD	2.35	0.43
2:B:782:ILE:HB	2:B:798:PRO:HB3	1.89	0.43
2:B:811:LEU:HG	2:B:813:LEU:CD1	2.46	0.43
2:B:850:PHE:HZ	2:B:886:GLN:HB2	1.83	0.43
2:B:950:PRO:O	2:B:951:ASP:HB2	2.18	0.43
2:B:1023:ALA:O	2:B:1027:ILE:HG13	2.18	0.43
2:B:1069:ASN:HD22	2:B:1069:ASN:HA	1.55	0.43
2:B:1259:GLN:NE2	2:B:1262:LYS:CE	2.72	0.43
2:B:1260:TYR:CD2	2:B:1260:TYR:C	2.97	0.43
1:A:109:PHE:O	1:A:127:ILE:HG23	2.18	0.43
1:A:541:LEU:CG	2:B:796:ALA:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLN:O	1:A:594:ILE:N	2.50	0.43
1:A:617:PHE:CB	1:A:632:THR:HG21	2.47	0.43
2:B:1143:LEU:HD11	2:B:1147:ILE:CG1	2.49	0.43
2:B:1252:MET:C	2:B:1254:PHE:H	2.24	0.43
1:A:35:VAL:HG12	1:A:36:THR:N	2.33	0.43
1:A:358:ASP:OD1	1:A:358:ASP:N	2.52	0.43
1:A:365:VAL:CG1	1:A:379:THR:OG1	2.66	0.43
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.36	0.43
2:B:1121:LEU:O	2:B:1121:LEU:HD12	2.18	0.43
2:B:1217:ALA:C	2:B:1219:LEU:N	2.76	0.43
1:A:132:HIS:C	1:A:133:LYS:HG3	2.43	0.43
1:A:341:TYR:HB2	1:A:609:SER:CB	2.32	0.43
1:A:580:VAL:HG22	2:B:747:GLU:HG2	2.01	0.43
2:B:963:THR:HG22	2:B:963:THR:O	2.18	0.43
2:B:992:ASN:OD1	2:B:1033:GLN:NE2	2.52	0.43
1:A:117:TYR:CD2	1:A:200:PHE:CD1	3.07	0.43
1:A:118:THR:HB	2:B:815:TYR:CE1	2.54	0.43
1:A:131:ASN:C	1:A:133:LYS:H	2.27	0.43
1:A:443:LEU:CD1	1:A:449:LEU:HD22	2.42	0.43
2:B:744:GLU:HG3	2:B:774:LYS:CB	2.48	0.43
2:B:1336:CYS:O	2:B:1337:ASN:C	2.62	0.43
1:A:14:LEU:HD21	1:A:101:VAL:HG11	1.97	0.43
1:A:206:VAL:O	1:A:208:PRO:HD3	2.19	0.43
1:A:363:TYR:CE1	1:A:364:ARG:HD3	2.28	0.43
1:A:473:MET:O	1:A:474:ASN:HB2	2.18	0.43
2:B:975:ALA:HB2	2:B:1006:LEU:HD21	1.99	0.43
2:B:981:LEU:HD22	2:B:998:PRO:CB	2.49	0.43
1:A:58:THR:O	1:A:61:MET:N	2.52	0.43
1:A:103:LEU:CG	1:A:193:GLN:HE21	2.31	0.43
1:A:110:ILE:HG12	1:A:127:ILE:HG13	2.01	0.43
1:A:148:PRO:HB3	1:A:181:GLN:H	1.83	0.43
1:A:183:LYS:HA	1:A:199:GLU:HG2	2.01	0.43
1:A:335:PHE:CD2	1:A:419:MET:HB3	2.54	0.43
1:A:541:LEU:HD12	1:A:542:VAL:H	1.83	0.43
2:B:738:ASN:HD22	3:M:45:LYS:HE2	1.84	0.43
2:B:847:ASN:HA	2:B:848:PRO:HD2	1.90	0.43
2:B:1122:THR:O	2:B:1122:THR:HG22	2.18	0.43
2:B:1130:GLN:HE22	2:B:1177:MET:HE2	1.79	0.43
2:B:1153:PHE:CD2	2:B:1154:LEU:HD23	2.53	0.43
2:B:1163:ARG:C	2:B:1165:TYR:N	2.75	0.43
1:A:52:THR:HG23	1:A:53:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:CB	1:A:136:PRO:HD2	2.49	0.42
2:B:744:GLU:CB	2:B:775:ASP:HB2	2.42	0.42
2:B:974:ASP:O	2:B:976:GLU:N	2.52	0.42
2:B:1148:THR:O	2:B:1152:ASP:CG	2.62	0.42
2:B:1221:LEU:C	2:B:1222:LYS:HG3	2.44	0.42
2:B:1227:VAL:O	2:B:1231:VAL:HG23	2.19	0.42
1:A:78:LYS:HE3	1:A:82:LYS:HZ1	1.84	0.42
1:A:400:ILE:HD13	1:A:419:MET:HE3	2.00	0.42
1:A:555:PRO:CG	2:B:777:ILE:HG12	2.49	0.42
1:A:567:HIS:CB	2:B:760:PRO:HG3	2.46	0.42
1:A:12:LEU:HD12	1:A:84:VAL:HG21	2.01	0.42
1:A:34:THR:HG22	1:A:51:LYS:CE	2.49	0.42
1:A:144:ASN:ND2	1:A:155:GLN:HB3	2.34	0.42
1:A:269:ILE:HD12	1:A:277:GLU:C	2.44	0.42
1:A:470:TYR:HA	1:A:510:VAL:O	2.19	0.42
2:B:917:ASN:CB	2:B:1325:MET:HE2	2.30	0.42
2:B:927:PRO:HG2	2:B:1313:GLU:N	2.34	0.42
2:B:1054:THR:HG22	2:B:1054:THR:O	2.18	0.42
2:B:1217:ALA:O	2:B:1218:LEU:C	2.62	0.42
2:B:1341:LEU:HD23	2:B:1469:ARG:HB2	2.00	0.42
1:A:187:TYR:HB3	1:A:195:VAL:HA	2.00	0.42
1:A:223:ILE:HD12	1:A:223:ILE:H	1.85	0.42
1:A:350:LEU:N	1:A:351:MET:HE2	2.35	0.42
1:A:404:THR:CG2	1:A:414:GLN:HE21	2.26	0.42
2:B:1078:LEU:HD11	2:B:1132:ALA:CB	2.49	0.42
3:M:67:LYS:O	3:M:67:LYS:HG2	2.19	0.42
2:B:819:ARG:O	2:B:820:ASN:CB	2.65	0.42
2:B:1306:GLU:OE1	2:B:1306:GLU:HA	2.20	0.42
1:A:126:ARG:HG3	2:B:751:TRP:HZ2	1.84	0.42
1:A:280:LEU:HD11	1:A:284:VAL:HB	2.01	0.42
1:A:562:LYS:C	1:A:563:ILE:HG13	2.45	0.42
2:B:1107:MET:HB2	2:B:1247:THR:HB	2.01	0.42
3:M:37:ASN:ND2	3:M:38:THR:H	2.17	0.42
1:A:12:LEU:C	1:A:13:ARG:HG3	2.45	0.42
1:A:366:PRO:HG2	1:A:406:LYS:HA	2.01	0.42
1:A:613:TYR:O	1:A:617:PHE:CE2	2.72	0.42
1:A:432:ASN:O	1:A:525:VAL:HG11	2.19	0.42
2:B:749:TRP:CE3	2:B:750:LEU:CB	3.01	0.42
2:B:836:GLN:HG2	2:B:897:HIS:CE1	2.55	0.42
2:B:740:VAL:CB	3:M:42:ARG:HB2	2.44	0.42
2:B:744:GLU:H	2:B:775:ASP:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1063:VAL:O	2:B:1063:VAL:CG1	2.68	0.42
2:B:1113:ASN:O	2:B:1115:ASN:N	2.52	0.42
2:B:1132:ALA:HA	2:B:1135:ILE:HD12	2.01	0.42
2:B:1193:LYS:O	2:B:1194:ASP:HB2	2.20	0.42
2:B:1222:LYS:C	2:B:1224:PHE:CE2	2.98	0.42
1:A:47:LEU:HD21	1:A:49:SER:OG	2.20	0.42
1:A:194:GLN:NE2	1:A:196:PHE:HE1	2.18	0.42
1:A:522:ARG:HD2	1:A:522:ARG:HA	1.51	0.42
1:A:555:PRO:O	3:M:42:ARG:NH2	2.52	0.42
2:B:818:VAL:HG12	2:B:819:ARG:N	2.35	0.42
2:B:1115:ASN:HB3	2:B:1163:ARG:HD2	2.02	0.42
2:B:774:LYS:HB2	2:B:780:TRP:CZ2	2.54	0.41
2:B:1277:GLN:O	2:B:1308:PHE:HB2	2.20	0.41
1:A:103:LEU:HG	1:A:193:GLN:NE2	2.32	0.41
1:A:113:ASP:OD2	2:B:748:SER:HB2	2.19	0.41
1:A:574:VAL:HG21	2:B:751:TRP:CZ3	2.54	0.41
2:B:1140:VAL:HG13	2:B:1142:SER:H	1.84	0.41
1:A:164:LEU:HD23	1:A:570:ARG:CB	2.50	0.41
1:A:369:VAL:HG12	1:A:370:GLN:N	2.35	0.41
1:A:375:VAL:HG22	1:A:387:LEU:HD21	2.02	0.41
1:A:537:CYS:O	1:A:537:CYS:SG	2.77	0.41
1:A:580:VAL:CG2	2:B:747:GLU:CB	2.97	0.41
2:B:981:LEU:CD1	2:B:1002:ALA:HB2	2.50	0.41
2:B:1014:LYS:H	2:B:1014:LYS:HG2	1.64	0.41
2:B:1105:GLN:O	2:B:1112:ARG:NE	2.53	0.41
1:A:427:VAL:C	1:A:429:ASN:N	2.71	0.41
1:A:429:ASN:OD1	1:A:429:ASN:O	2.39	0.41
1:A:530:TRP:CE3	1:A:607:PRO:CB	3.01	0.41
1:A:554:VAL:CG1	1:A:555:PRO:CD	2.95	0.41
1:A:603:ILE:O	1:A:635:ARG:NH1	2.40	0.41
2:B:1086:ILE:CG2	2:B:1142:SER:HB2	2.51	0.41
2:B:1437:LEU:O	2:B:1438:ALA:HB2	2.20	0.41
2:B:1462:ASN:C	2:B:1464:GLU:H	2.27	0.41
1:A:1:SER:N	1:A:2:PRO:CD	2.82	0.41
1:A:55:THR:HG22	1:A:56:PRO:HD2	2.02	0.41
1:A:176:LEU:HD22	2:B:915:ARG:CD	2.51	0.41
1:A:221:TYR:CZ	1:A:228:GLY:HA2	2.56	0.41
1:A:370:GLN:HE22	1:A:403:ARG:CZ	2.31	0.41
2:B:840:VAL:HG12	2:B:841:ARG:H	1.85	0.41
2:B:1204:GLN:HA	2:B:1207:ASN:ND2	2.35	0.41
2:B:1274:VAL:HG22	2:B:1312:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1366:ILE:HD13	2:B:1455:VAL:CG1	2.48	0.41
3:M:44:ILE:HD12	3:M:77:ILE:HD12	2.02	0.41
1:A:153:VAL:HG21	1:A:171:TRP:CZ2	2.55	0.41
1:A:218:GLU:HB3	1:A:220:PHE:O	2.21	0.41
1:A:311:HIS:HA	2:B:1423:ILE:HD11	2.02	0.41
1:A:315:ASP:OD1	1:A:316:MET:N	2.53	0.41
1:A:477:ARG:NH1	1:A:479:LEU:HD13	2.35	0.41
1:A:593:LYS:O	1:A:597:VAL:HG23	2.21	0.41
2:B:1106:GLU:HA	2:B:1112:ARG:NH1	2.35	0.41
2:B:1230:VAL:CG1	2:B:1230:VAL:O	2.66	0.41
3:M:52:MET:HE3	3:M:52:MET:HB2	1.70	0.41
2:B:991:GLN:CD	2:B:1104:HIS:CE1	2.98	0.41
2:B:1192:ALA:HB1	2:B:1195:LYS:HA	2.03	0.41
2:B:1253:VAL:O	2:B:1253:VAL:HG22	2.20	0.41
3:M:53:TYR:CD2	3:M:53:TYR:C	2.98	0.41
1:A:61:MET:HG3	1:A:483:ARG:CZ	2.51	0.41
1:A:168:PRO:C	1:A:169:LEU:HG	2.45	0.41
1:A:220:PHE:CE1	1:A:330:PRO:HG3	2.56	0.41
1:A:269:ILE:HD13	1:A:278:VAL:HB	2.03	0.41
2:B:942:PRO:HG3	2:B:1307:GLY:CA	2.51	0.41
2:B:990:GLU:O	2:B:994:ILE:HG13	2.19	0.41
2:B:1061:VAL:HG12	2:B:1061:VAL:O	2.21	0.41
2:B:1161:LEU:HD13	2:B:1166:THR:O	2.20	0.41
2:B:1252:MET:C	2:B:1254:PHE:N	2.79	0.41
2:B:1446:ASN:O	2:B:1447:VAL:HG23	2.21	0.41
1:A:153:VAL:HG21	1:A:171:TRP:CH2	2.56	0.41
1:A:163:GLN:HE21	1:A:163:GLN:HB2	1.65	0.41
1:A:344:PRO:HD2	1:A:433:TYR:CE1	2.55	0.41
1:A:536:SER:O	1:A:595:TRP:CZ2	2.74	0.41
1:A:549:GLU:O	1:A:549:GLU:HG2	2.21	0.41
1:A:558:GLN:CD	3:M:40:TYR:OH	2.63	0.41
2:B:742:ARG:H	2:B:903:VAL:HA	1.86	0.41
2:B:744:GLU:CA	2:B:746:PRO:HD2	2.50	0.41
2:B:782:ILE:HD11	2:B:799:PHE:CZ	2.55	0.41
2:B:799:PHE:HE1	2:B:801:VAL:CG2	2.31	0.41
2:B:817:VAL:HG21	2:B:907:LEU:HD11	2.01	0.41
2:B:1408:SER:O	2:B:1410:TYR:N	2.54	0.41
3:M:67:LYS:O	3:M:71:GLN:HB2	2.20	0.41
1:A:4:TYR:O	1:A:627:SER:HB3	2.21	0.41
1:A:213:ILE:HG22	1:A:215:GLU:HG3	2.03	0.41
1:A:370:GLN:OE1	1:A:403:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:HG22	1:A:387:LEU:CD2	2.51	0.41
1:A:468:TYR:HE2	1:A:486:ARG:HB2	1.85	0.41
2:B:1083:LYS:HD2	2:B:1140:VAL:HG22	2.03	0.41
2:B:1119:MET:HE3	2:B:1119:MET:HB3	1.90	0.41
1:A:166:VAL:O	1:A:167:LEU:HD23	2.21	0.40
1:A:361:PRO:CB	1:A:383:GLY:HA3	2.50	0.40
1:A:474:ASN:O	1:A:475:LYS:HB2	2.22	0.40
1:A:502:ASP:OD1	1:A:502:ASP:N	2.54	0.40
1:A:577:ASP:C	1:A:579:GLY:H	2.28	0.40
2:B:967:GLN:O	2:B:968:MET:C	2.64	0.40
2:B:1341:LEU:HD11	2:B:1366:ILE:CG2	2.51	0.40
3:M:37:ASN:C	3:M:39:TYR:H	2.28	0.40
3:M:84:LYS:O	3:M:84:LYS:HG3	2.21	0.40
1:A:63:ASN:HB3	4:A:646:NAG:C1	2.52	0.40
1:A:142:MET:SD	1:A:142:MET:N	2.94	0.40
1:A:242:LYS:HD3	1:A:273:ASP:O	2.21	0.40
1:A:640:CYS:HB3	1:A:641:PRO:CD	2.51	0.40
2:B:975:ALA:HB1	2:B:1006:LEU:HD21	1.98	0.40
2:B:1016:GLY:C	2:B:1018:GLU:H	2.28	0.40
2:B:1085:LEU:HD13	2:B:1125:VAL:CG1	2.51	0.40
1:A:63:ASN:HB2	4:A:646:NAG:H2	2.03	0.40
1:A:110:ILE:HD12	1:A:198:THR:HB	2.03	0.40
1:A:124:LEU:HD23	1:A:169:LEU:O	2.20	0.40
1:A:543:VAL:O	2:B:799:PHE:CD2	2.74	0.40
1:A:582:VAL:O	1:A:582:VAL:CG1	2.69	0.40
2:B:855:THR:OG1	2:B:858:ARG:NH1	2.55	0.40
2:B:985:PRO:CD	2:B:1026:LEU:HB3	2.48	0.40
2:B:1003:VAL:CG1	2:B:1070:LEU:HD22	2.51	0.40
2:B:1198:TRP:O	2:B:1210:ALA:HB3	2.21	0.40
2:B:1213:TYR:CD1	2:B:1216:LEU:HD12	2.56	0.40
2:B:1399:LEU:O	2:B:1405:ARG:HB3	2.20	0.40
3:M:77:ILE:O	3:M:77:ILE:HG22	2.21	0.40
1:A:117:TYR:CE2	1:A:123:VAL:HG13	2.57	0.40
1:A:154:LYS:CD	1:A:171:TRP:CD1	3.03	0.40
1:A:386:LYS:HA	1:A:386:LYS:HD2	1.69	0.40
1:A:430:SER:C	1:A:431:ASN:OD1	2.63	0.40
2:B:1026:LEU:HA	2:B:1029:LYS:HB3	2.02	0.40
2:B:1113:ASN:HD22	2:B:1163:ARG:CZ	2.33	0.40
2:B:1375:ASP:OD1	2:B:1375:ASP:N	2.55	0.40
1:A:176:LEU:HD22	2:B:915:ARG:HD3	2.02	0.40
1:A:363:TYR:CE2	1:A:381:GLY:HA2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1000:VAL:HG13	2:B:1070:LEU:CD1	2.51	0.40
2:B:1141:ASN:O	2:B:1144:PRO:HD2	2.21	0.40
2:B:1228:PRO:CB	2:B:1229:PRO:CD	2.87	0.40
2:B:1397:LYS:CE	2:B:1412:LEU:HG	2.49	0.40
3:M:50:LYS:CE	3:M:65:GLU:HG3	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	628/645 (97%)	524 (83%)	88 (14%)	16 (2%)	4	26
2	B	881/915 (96%)	726 (82%)	126 (14%)	29 (3%)	3	21
3	M	82/88 (93%)	73 (89%)	9 (11%)	0	100	100
All	All	1591/1648 (96%)	1323 (83%)	223 (14%)	45 (3%)	4	24

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	ASN
1	A	505	PRO
1	A	518	ALA
2	B	733	ILE
2	B	783	LEU
2	B	1270	LEU
1	A	20	MET
1	A	241	LYS
1	A	407	GLN
1	A	474	ASN
2	B	792	GLY
2	B	989	GLY

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Mol	Chain	Res	Type
2	B	1039	GLN
2	B	1218	LEU
2	B	1393	THR
2	B	1573	LYS
1	A	442	GLU
1	A	458	ASP
2	B	968	MET
2	B	1149	LYS
2	B	1486	ASP
1	A	620	ALA
1	A	638	LEU
2	B	1222	LYS
2	B	1571	ALA
1	A	271	ILE
1	A	641	PRO
2	B	782	ILE
2	B	820	ASN
2	B	848	PRO
2	B	926	ASP
2	B	954	SER
2	B	1175	ALA
2	B	1409	LYS
1	A	640	CYS
2	B	953	GLU
2	B	1114	ASN
2	B	1238	ARG
2	B	1337	ASN
1	A	145	ILE
2	B	880	PRO
2	B	1453	GLY
1	A	393	PRO
2	B	1016	GLY
2	B	1452	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	557/567 (98%)	498 (89%)	59 (11%)	6	21
2	B	790/810 (98%)	712 (90%)	78 (10%)	7	24
3	M	76/79 (96%)	71 (93%)	5 (7%)	15	37
All	All	1423/1456 (98%)	1281 (90%)	142 (10%)	7	24

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	8	THR
1	A	20	MET
1	A	52	THR
1	A	55	THR
1	A	61	MET
1	A	92	THR
1	A	103	LEU
1	A	105	SER
1	A	113	ASP
1	A	122	THR
1	A	125	TYR
1	A	130	VAL
1	A	142	MET
1	A	155	GLN
1	A	177	VAL
1	A	179	MET
1	A	193	GLN
1	A	194	GLN
1	A	239	TYR
1	A	261	SER
1	A	301	SER
1	A	327	VAL
1	A	328	THR
1	A	331	TYR
1	A	346	MET
1	A	350	LEU
1	A	351	MET
1	A	355	THR
1	A	375	VAL
1	A	378	LEU
1	A	389	ILE
1	A	398	LEU
1	A	399	SER

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Mol	Chain	Res	Type
1	A	425	SER
1	A	430	SER
1	A	437	SER
1	A	438	VAL
1	A	439	LEU
1	A	452	ASN
1	A	453	PHE
1	A	458	ASP
1	A	459	ARG
1	A	477	ARG
1	A	479	LEU
1	A	480	LYS
1	A	485	VAL
1	A	487	GLU
1	A	495	LEU
1	A	502	ASP
1	A	509	LEU
1	A	515	LEU
1	A	519	SER
1	A	522	ARG
1	A	554	VAL
1	A	573	LEU
1	A	574	VAL
1	A	616	VAL
1	A	639	GLN
2	B	747	GLU
2	B	757	LYS
2	B	758	GLU
2	B	762	ASN
2	B	770	ASN
2	B	776	SER
2	B	789	ASP
2	B	828	VAL
2	B	833	ARG
2	B	834	GLN
2	B	845	LEU
2	B	851	CYS
2	B	885	LEU
2	B	907	LEU
2	B	912	GLU
2	B	917	ASN
2	B	935	VAL

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Mol	Chain	Res	Type
2	B	937	LYS
2	B	940	ILE
2	B	945	LEU
2	B	951	ASP
2	B	953	GLU
2	B	968	MET
2	B	976	GLU
2	B	977	ARG
2	B	978	LEU
2	B	982	ILE
2	B	990	GLU
2	B	1018	GLU
2	B	1033	GLN
2	B	1060	VAL
2	B	1069	ASN
2	B	1078	LEU
2	B	1099	ASP
2	B	1117	LYS
2	B	1136	CYS
2	B	1137	GLU
2	B	1139	GLN
2	B	1141	ASN
2	B	1196	ASN
2	B	1259	GLN
2	B	1262	LYS
2	B	1268	GLN
2	B	1269	GLU
2	B	1281	ARG
2	B	1282	SER
2	B	1283	SER
2	B	1284	LYS
2	B	1292	GLU
2	B	1301	GLU
2	B	1303	LYS
2	B	1334	LEU
2	B	1337	ASN
2	B	1342	LYS
2	B	1361	THR
2	B	1377	THR
2	B	1384	SER
2	B	1387	THR
2	B	1393	THR

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Mol	Chain	Res	Type
2	B	1396	LEU
2	B	1397	LYS
2	B	1411	GLU
2	B	1412	LEU
2	B	1419	ARG
2	B	1423	ILE
2	B	1433	GLU
2	B	1447	VAL
2	B	1448	GLU
2	B	1462	ASN
2	B	1483	LEU
2	B	1487	GLU
2	B	1488	LEU
2	B	1489	CYS
2	B	1498	ILE
2	B	1503	ASP
2	B	1535	ASP
2	B	1569	ARG
2	B	1637	PHE
3	M	11	GLN
3	M	23	LEU
3	M	56	LYS
3	M	69	GLN
3	M	71	GLN

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

Mol	Chain	Res	Type
1	A	63	ASN
1	A	87	GLN
1	A	104	GLN
1	A	132	HIS
1	A	144	ASN
1	A	155	GLN
1	A	162	ASN
1	A	163	GLN
1	A	193	GLN
1	A	194	GLN
1	A	318	GLN
1	A	380	GLN
1	A	390	ASN
1	A	414	GLN

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Mol	Chain	Res	Type
1	A	420	GLN
1	A	435	HIS
1	A	490	GLN
1	A	558	GLN
1	A	567	HIS
1	A	587	ASN
1	A	631	GLN
1	A	634	GLN
1	A	639	GLN
2	B	738	ASN
2	B	770	ASN
2	B	820	ASN
2	B	834	GLN
2	B	847	ASN
2	B	862	GLN
2	B	886	GLN
2	B	897	HIS
2	B	948	GLN
2	B	992	ASN
2	B	1033	GLN
2	B	1069	ASN
2	B	1076	GLN
2	B	1090	GLN
2	B	1104	HIS
2	B	1113	ASN
2	B	1115	ASN
2	B	1160	ASN
2	B	1176	GLN
2	B	1196	ASN
2	B	1204	GLN
2	B	1259	GLN
2	B	1261	GLN
2	B	1267	HIS
2	B	1277	GLN
2	B	1431	HIS
2	B	1442	HIS
2	B	1451	GLN
2	B	1462	ASN
3	M	11	GLN
3	M	37	ASN
3	M	49	GLN
3	M	69	GLN

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Mol	Chain	Res	Type
3	M	71	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	NAG	A	647	-	14,14,15	0.62	0	17,19,21	1.69	4 (23%)
5	MAN	A	648	-	11,11,12	0.70	0	15,15,17	0.50	0
4	NAG	A	649	-	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
4	NAG	A	646	-	14,14,15	0.59	0	17,19,21	1.84	5 (29%)

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
4	NAG	A	647	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	648	-	-	0/2/19/22	0/1/1/1
4	NAG	A	649	-	-	2/6/23/26	0/1/1/1
4	NAG	A	646	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	647	NAG	C4-C3-C2	4.22	117.20	111.02
4	A	646	NAG	C2-N2-C7	4.19	128.51	122.90
4	A	647	NAG	C3-C4-C5	3.42	116.44	110.23
4	A	646	NAG	C8-C7-N2	3.32	121.63	116.12
4	A	646	NAG	C1-C2-N2	3.16	115.42	110.43
4	A	646	NAG	O5-C5-C6	2.96	113.42	107.66
4	A	647	NAG	C1-O5-C5	-2.81	108.42	112.19
4	A	646	NAG	O7-C7-C8	-2.22	118.11	122.05
4	A	649	NAG	O5-C1-C2	2.14	114.60	111.29
4	A	647	NAG	O5-C1-C2	-2.07	108.09	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	646	NAG	C8-C7-N2-C2
4	A	646	NAG	O7-C7-N2-C2
4	A	646	NAG	O5-C5-C6-O6
4	A	646	NAG	C4-C5-C6-O6
4	A	649	NAG	C8-C7-N2-C2
4	A	649	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	647	NAG	2	0
5	A	648	MAN	1	0
4	A	646	NAG	4	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	634/645 (98%)	0.22	58 (9%)	15 22	60, 127, 187, 245	0
2	B	748/915 (81%)	0.21	63 (8%)	17 24	20, 180, 248, 326	0
3	M	84/88 (95%)	-0.09	3 (3%)	46 43	165, 204, 265, 298	0
All	All	1466/1648 (88%)	0.20	124 (8%)	16 24	20, 156, 238, 326	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1439	PHE	7.7
2	B	825	ILE	7.2
2	B	1257	LEU	6.5
2	B	842	VAL	6.5
1	A	480	LYS	5.6
2	B	892	ALA	5.5
2	B	1391	PRO	5.1
2	B	864	VAL	4.9
2	B	782	ILE	4.8
1	A	439	LEU	4.7
1	A	449	LEU	4.5
2	B	827	ALA	4.4
2	B	824	GLU	4.4
2	B	1221	LEU	4.4
2	B	1219	LEU	4.2
2	B	840	VAL	4.2
1	A	511	ALA	4.1
1	A	20	MET	4.1
1	A	527	ASP	4.0
2	B	1101	PRO	4.0
1	A	470	TYR	3.9
1	A	491	ASP	3.8
1	A	512	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	1204	GLN	3.8
1	A	472	ILE	3.7
1	A	436	LEU	3.7
1	A	468	TYR	3.6
2	B	1256	ALA	3.5
2	B	1082	VAL	3.5
1	A	86	VAL	3.5
2	B	823	VAL	3.5
2	B	745	PHE	3.4
1	A	440	ARG	3.3
2	B	1251	PHE	3.3
1	A	471	LEU	3.3
1	A	532	ASP	3.3
2	B	1254	PHE	3.3
1	A	497	LEU	3.3
2	B	1263	ASP	3.2
2	B	874	VAL	3.2
1	A	22	LEU	3.2
2	B	1156	ALA	3.1
2	B	1213	TYR	3.0
2	B	1218	LEU	3.0
2	B	1010	GLU	3.0
2	B	810	ASP	3.0
1	A	434	LEU	3.0
2	B	1364	LEU	3.0
1	A	438	VAL	3.0
1	A	453	PHE	3.0
1	A	509	LEU	2.9
2	B	876	TYR	2.9
1	A	526	ALA	2.9
2	B	1203	LYS	2.9
3	M	38	THR	2.9
2	B	1282	SER	2.9
2	B	1437	LEU	2.9
1	A	125	TYR	2.9
2	B	811	LEU	2.9
1	A	162	ASN	2.9
1	A	297	LEU	2.8
1	A	454	LEU	2.8
2	B	769	MET	2.8
1	A	21	VAL	2.8
2	B	1304	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	444	ARG	2.7
1	A	628	SER	2.7
2	B	829	LEU	2.7
2	B	1360	ASN	2.6
2	B	1223	ASP	2.6
2	B	1201	PRO	2.6
1	A	251	PHE	2.6
1	A	78	LYS	2.6
1	A	169	LEU	2.5
2	B	1243	GLY	2.5
1	A	389	ILE	2.5
2	B	1424	ILE	2.5
1	A	175	GLU	2.5
1	A	121	SER	2.5
2	B	1381	LEU	2.5
1	A	451	VAL	2.4
1	A	109	PHE	2.4
2	B	770	ASN	2.4
1	A	285	LEU	2.4
1	A	318	GLN	2.4
1	A	79	GLY	2.4
2	B	1366	ILE	2.4
1	A	289	VAL	2.4
2	B	1244	TYR	2.4
1	A	120	GLY	2.3
2	B	1280	SER	2.3
1	A	7	ILE	2.3
1	A	84	VAL	2.3
1	A	6	ILE	2.3
1	A	500	THR	2.3
2	B	1092	PRO	2.3
3	M	83	SER	2.3
2	B	1117	LYS	2.3
2	B	890	VAL	2.3
1	A	641	PRO	2.3
2	B	784	ALA	2.2
2	B	983	VAL	2.2
1	A	382	ASP	2.2
1	A	510	VAL	2.2
2	B	953	GLU	2.2
2	B	809	ILE	2.2
2	B	1390	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1217	ALA	2.2
2	B	958	ILE	2.2
1	A	313	GLY	2.1
2	B	791	LYS	2.1
2	B	1348	ALA	2.1
1	A	82	LYS	2.1
2	B	1396	LEU	2.1
1	A	37	VAL	2.1
3	M	29	ASN	2.1
1	A	551	ARG	2.1
2	B	748	SER	2.0
1	A	398	LEU	2.0
2	B	878	ILE	2.0
1	A	133	LYS	2.0
1	A	481	ALA	2.0
2	B	1242	GLY	2.0
1	A	543	VAL	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 ⓘ

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
5	MAN	A	648	11/12	-0.55	0.22	211,220,230,239	0
4	NAG	A	649	14/15	0.42	0.29	198,208,218,226	0
4	NAG	A	646	14/15	0.87	0.13	117,151,158,160	0
4	NAG	A	647	14/15	0.89	0.11	154,188,202,211	0

6.5 Other polymers [i](#)

There are no such residues in this entry.