



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:07 AM UTC

PDB ID : 2WQZ / pdb_00002wqz
Title : Crystal structure of synaptic protein neuroligin-4 in complex with neurexin-beta 1: alternative refinement
Authors : Fabrichny, I.P.; Leone, P.; Sulzenbacher, G.; Comoletti, D.; Miller, M.T.; Taylor, P.; Bourne, Y.; Marchot, P.
Deposited on : 2009-08-28
Resolution : 3.90 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

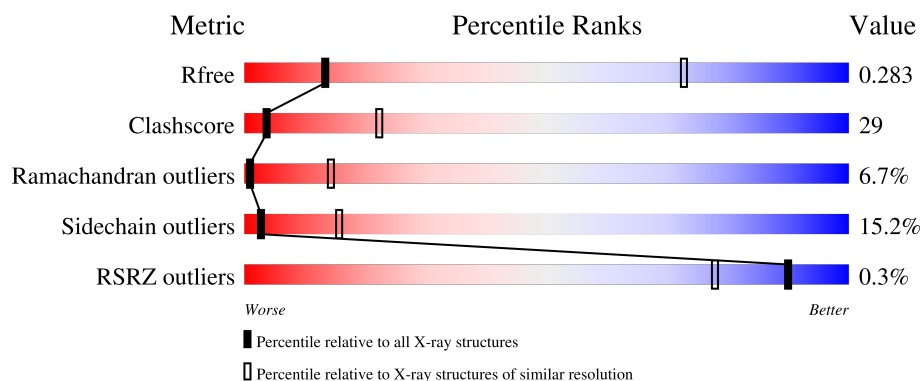
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	588	
1	B	588	
2	C	179	
2	D	179	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11360 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 NEUROLIGIN 4, X-LINKED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4310	2756	712	821	21			
1	B	544	Total	C	N	O	S	0	0	0
			4302	2749	713	819	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	561	ARG	LYS	conflict	UNP Q8N0W4
B	561	ARG	LYS	conflict	UNP Q8N0W4

- Molecule 2 is a protein called NEUREXIN-1-BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	D	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

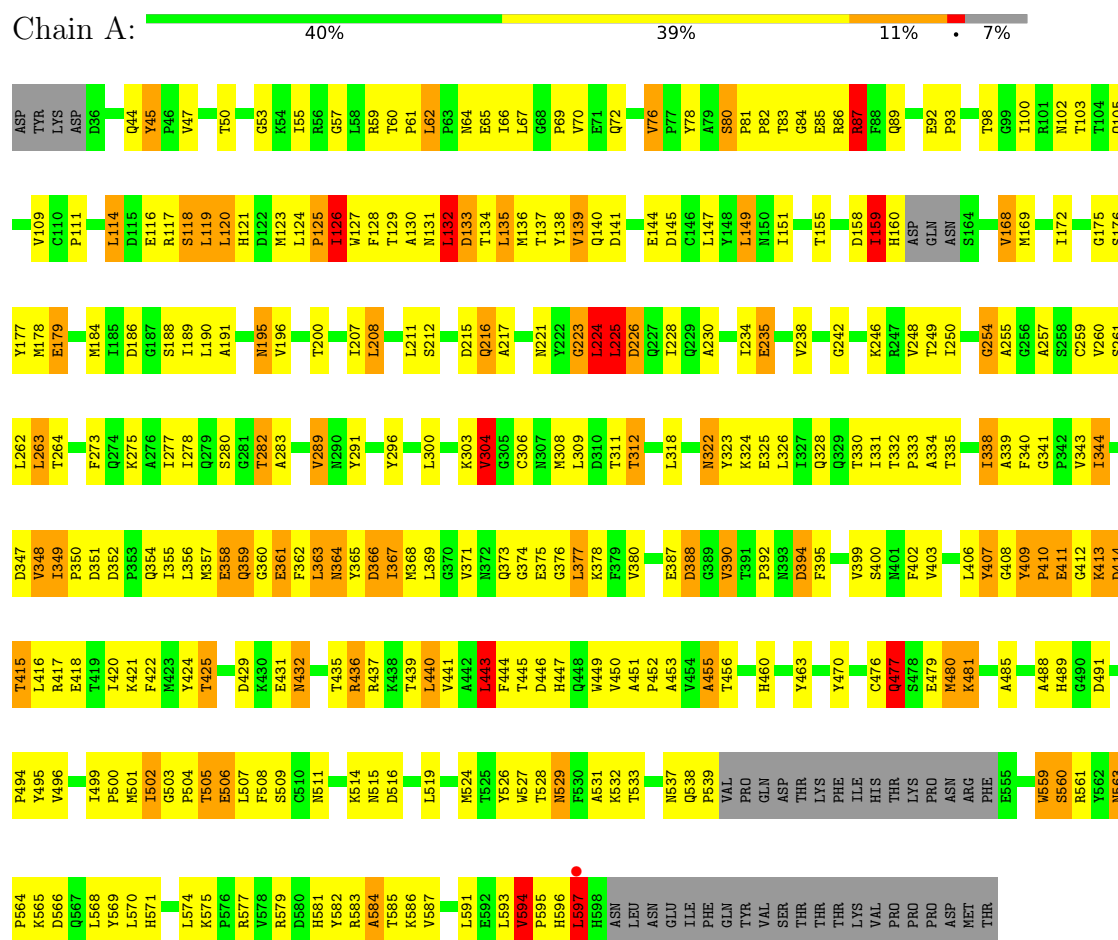
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

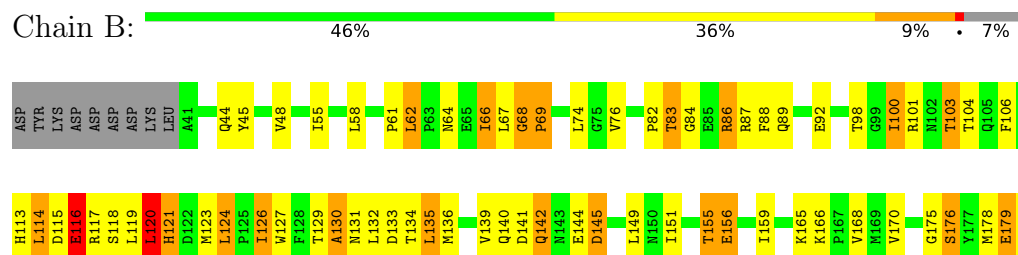
3 Residue-property plots

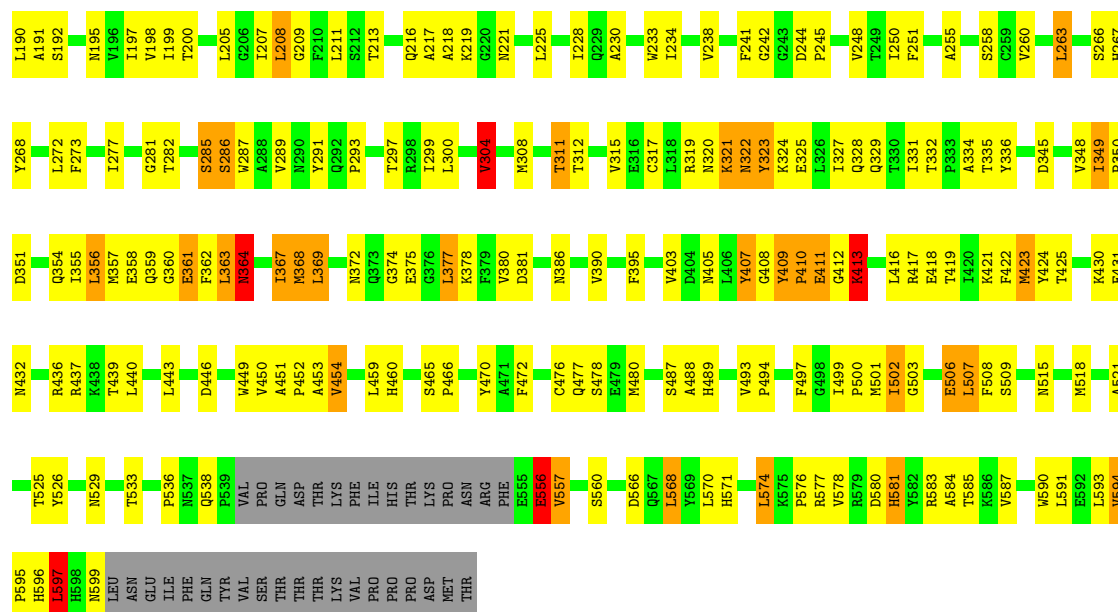
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NEUROLIGIN 4, X-LINKED

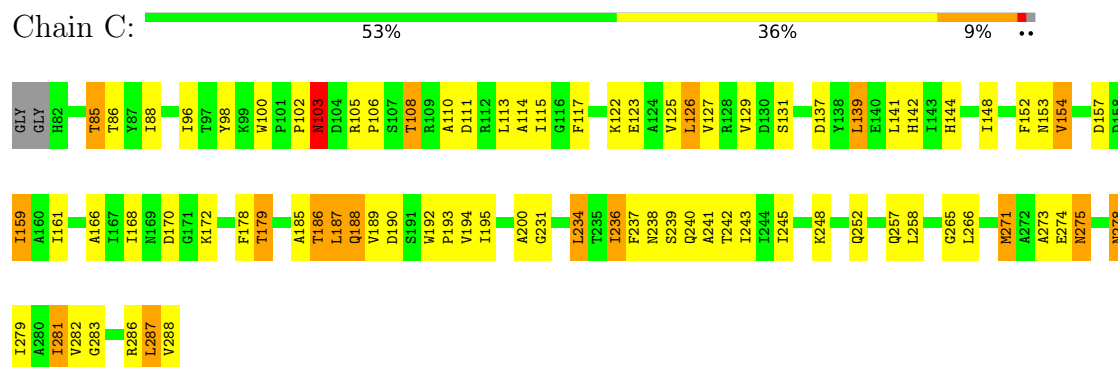


• Molecule 1: NEUROLIGIN 4, X-LINKED

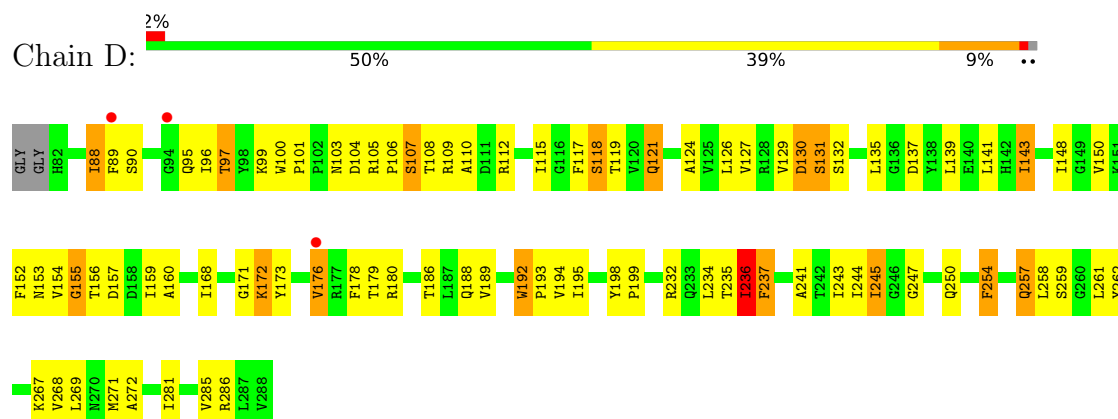




• Molecule 2: NEUREXIN-1-BETA



• Molecule 2: NEUREXIN-1-BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	158.52Å 198.67Å 85.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.90 30.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.90) 99.2 (30.00-3.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.205 , 0.276 0.212 , 0.283	Depositor DCC
R_{free} test set	2178 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	92.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 115.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11360	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, CA

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	0.70	1/4429 (0.0%)	0.95	8/6040 (0.1%)
1	B	0.68	0/4422	0.94	13/6033 (0.2%)
2	C	0.61	0/1384	0.82	0/1874
2	D	0.90	2/1384 (0.1%)	0.99	6/1874 (0.3%)
All	All	0.71	3/11619 (0.0%)	0.94	27/15821 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	176	VAL	CA-CB	6.27	1.60	1.53
2	D	245	ILE	CA-CB	5.55	1.59	1.53
1	A	347	ASP	CA-C	5.47	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	GLY	CA-C-N	10.20	132.59	119.84
1	A	503	GLY	C-N-CA	10.20	132.59	119.84
1	A	563	ASN	CA-C-N	8.06	129.92	119.84
1	A	563	ASN	C-N-CA	8.06	129.92	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	236	ILE	N-CA-C	7.76	118.98	108.11
1	B	349	ILE	CA-C-N	6.95	127.25	119.32
1	B	349	ILE	C-N-CA	6.95	127.25	119.32
2	D	90	SER	N-CA-C	6.82	118.56	108.60
1	B	110	CYS	CA-C-N	6.39	127.83	119.84
1	B	110	CYS	C-N-CA	6.39	127.83	119.84
1	B	322	ASN	N-CA-C	6.20	117.65	108.60
1	B	556	GLU	N-CA-C	6.00	123.59	110.80
1	A	455	ALA	N-CA-C	-5.98	102.48	110.55
1	B	68	GLY	CA-C-N	5.86	125.82	119.78
1	B	68	GLY	C-N-CA	5.86	125.82	119.78
1	A	361	GLU	N-CA-C	5.81	117.90	109.71
1	B	179	GLU	N-CA-C	5.41	117.24	108.26
1	B	597	LEU	N-CA-C	5.38	122.27	110.80
1	B	44	GLN	N-CA-C	5.32	117.16	111.36
2	D	259	SER	N-CA-C	5.30	116.58	108.42
1	A	538	GLN	N-CA-C	5.14	121.18	109.81
2	D	257	GLN	N-CA-C	5.13	115.12	107.88
1	A	362	PHE	N-CA-C	-5.11	101.64	109.41
1	B	69	PRO	N-CA-C	5.10	119.31	111.21
2	D	281	ILE	N-CA-C	5.08	114.60	106.88
2	D	121	GLN	N-CA-C	5.06	117.31	108.76
1	B	281	GLY	N-CA-C	5.01	116.92	110.96

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide
1	A	410	PRO	Peptide
1	A	411	GLU	Peptide
1	A	537	ASN	Peptide
1	A	597	LEU	Peptide
1	B	556	GLU	Peptide
1	B	596	HIS	Peptide
1	B	597	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4310	0	4133	283	0
1	B	4302	0	4122	225	0
2	C	1359	0	1346	73	0
2	D	1359	0	1346	90	0
3	A	28	0	26	8	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	11360	0	10973	651	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (651) 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:B:119:LEU:O	1:B:120:LEU:HD22	1.53	1.08
1:A:189:ILE:HD11	1:A:502:ILE:HD12	1.28	1.08
1:A:139:VAL:HG13	1:A:140:GLN:H	1.24	0.98
1:A:149:LEU:CD1	1:A:151:ILE:HD11	1.96	0.95
2:D:141:LEU:HD11	2:D:148:ILE:HG23	1.47	0.94
2:D:95:GLN:HE21	2:D:244:ILE:HG23	1.35	0.92
1:A:367:ILE:HD12	1:A:460:HIS:CE1	2.06	0.90
1:A:168:VAL:HG11	1:A:238:VAL:HG21	1.53	0.89
2:C:179:THR:OG1	2:C:186:THR:HG23	1.74	0.87
2:D:127:VAL:HG22	2:D:245:ILE:HG23	1.55	0.87
2:D:141:LEU:HD11	2:D:148:ILE:CG2	2.03	0.86
1:A:432:ASN:ND2	1:A:435:THR:OG1	2.09	0.86
1:B:597:LEU:HD21	1:B:599:ASN:HD22	1.41	0.86
1:B:361:GLU:HA	2:C:236:ILE:CD1	2.06	0.86
2:C:236:ILE:HD12	2:C:236:ILE:N	1.91	0.84
1:A:149:LEU:HD13	1:A:151:ILE:CD1	2.09	0.83
2:C:102:PRO:O	2:C:103:ASN:CG	2.22	0.83
1:A:149:LEU:HD13	1:A:151:ILE:HD11	1.61	0.82
2:D:95:GLN:NE2	2:D:244:ILE:HG23	1.94	0.82
1:A:175:GLY:H	1:A:255:ALA:HB3	1.47	0.80
1:B:361:GLU:HA	2:C:236:ILE:HD13	1.62	0.80
1:B:581:HIS:HB3	1:B:584:ALA:HB2	1.64	0.80
1:A:136:MET:O	1:A:139:VAL:HG12	1.82	0.80
1:B:360:GLY:O	1:B:362:PHE:N	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:GLY:O	1:B:410:PRO:HD3	1.82	0.79
1:B:151:ILE:HG21	1:B:241:PHE:HE1	1.49	0.78
2:C:127:VAL:HG22	2:C:245:ILE:HG23	1.65	0.78
1:A:300:LEU:HD12	1:A:331:ILE:HD11	1.65	0.78
1:B:114:LEU:HD13	1:B:132:LEU:HD22	1.66	0.77
1:B:250:ILE:CD1	1:B:263:LEU:HD11	2.15	0.77
1:B:234:ILE:O	1:B:238:VAL:HG12	1.84	0.77
1:A:169:MET:HE3	1:A:531:ALA:CB	2.14	0.77
1:B:129:THR:HG23	1:B:129:THR:O	1.82	0.77
1:A:111:PRO:HG3	1:A:208:LEU:HD12	1.67	0.76
1:B:507:LEU:HD22	1:B:508:PHE:CD1	2.20	0.76
1:A:149:LEU:HD11	1:A:151:ILE:HD11	1.68	0.76
2:C:236:ILE:HD12	2:C:236:ILE:H	1.51	0.75
2:C:129:VAL:HG12	2:C:243:ILE:HG12	1.69	0.75
1:A:581:HIS:HB3	1:A:584:ALA:HB2	1.68	0.75
1:A:131:ASN:ND2	1:A:135:LEU:HD21	2.00	0.75
1:A:277:ILE:CG2	1:A:368:MET:HE2	2.18	0.74
1:A:304:VAL:CG1	1:A:304:VAL:O	2.35	0.74
2:C:125:VAL:HG23	2:C:252:GLN:HE21	1.52	0.74
1:A:111:PRO:CG	1:A:208:LEU:HD12	2.16	0.74
1:A:277:ILE:HG23	1:A:368:MET:HE2	1.70	0.73
1:A:359:GLN:O	1:A:463:TYR:CE2	2.41	0.73
1:A:189:ILE:HD11	1:A:502:ILE:CD1	2.14	0.73
1:B:55:ILE:HB	1:B:103:THR:HG21	1.69	0.73
2:D:155:GLY:HA3	2:D:234:LEU:HD12	1.68	0.73
2:D:96:ILE:HG22	2:D:245:ILE:HB	1.70	0.72
1:B:367:ILE:CG2	1:B:369:LEU:HD22	2.19	0.72
1:B:129:THR:HG21	1:B:378:LYS:HE2	1.70	0.72
1:B:351:ASP:HB3	1:B:356:LEU:HD23	1.70	0.71
1:B:368:MET:CE	1:B:536:PRO:HG3	2.21	0.71
1:A:114:LEU:HD22	1:A:114:LEU:H	1.55	0.71
1:A:86:ARG:NH1	1:A:92:GLU:OE1	2.24	0.71
1:A:505:THR:CG2	1:A:508:PHE:HB2	2.21	0.70
1:A:526:TYR:HE2	1:A:570:LEU:HD21	1.57	0.70
1:B:139:VAL:HG12	1:B:139:VAL:O	1.91	0.70
1:A:390:VAL:O	1:A:436:ARG:NH1	2.24	0.70
2:D:126:LEU:HD23	2:D:143:ILE:HD11	1.73	0.70
2:D:143:ILE:HG22	2:D:143:ILE:O	1.91	0.70
1:B:250:ILE:HD11	1:B:263:LEU:HD11	1.73	0.69
1:A:304:VAL:O	1:A:304:VAL:HG13	1.92	0.69
1:A:102:ASN:ND2	3:A:1599:NAG:H2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:GLU:O	1:B:413:LYS:N	2.25	0.69
2:C:287:LEU:HD12	2:C:287:LEU:H	1.57	0.69
2:D:131:SER:O	2:D:241:ALA:HB3	1.93	0.68
1:A:413:LYS:O	1:A:416:LEU:N	2.26	0.68
1:A:207:ILE:HD11	1:A:300:LEU:CD1	2.23	0.68
1:A:402:PHE:CE1	1:A:406:LEU:HD12	2.29	0.68
1:A:66:ILE:O	1:A:66:ILE:HD12	1.94	0.68
1:B:250:ILE:HG12	1:B:260:VAL:HG13	1.75	0.68
1:B:367:ILE:HG23	1:B:369:LEU:HD22	1.74	0.68
1:B:114:LEU:CD1	1:B:132:LEU:HD22	2.24	0.68
2:C:152:PHE:CZ	2:C:159:ILE:HD12	2.29	0.67
1:A:207:ILE:HD11	1:A:300:LEU:HD11	1.75	0.67
2:C:189:VAL:HG12	2:C:190:ASP:OD2	1.94	0.67
2:C:117:PHE:CZ	2:C:168:ILE:HD13	2.29	0.67
1:A:324:LYS:O	1:A:326:LEU:N	2.26	0.67
1:B:121:HIS:HA	1:B:124:LEU:HG	1.76	0.67
2:C:98:TYR:O	2:C:242:THR:HA	1.95	0.67
1:A:131:ASN:HB3	1:A:135:LEU:HD11	1.77	0.67
2:D:261:LEU:HD23	2:D:262:TYR:N	2.11	0.66
1:B:507:LEU:C	1:B:507:LEU:HD23	2.21	0.66
1:A:376:GLY:O	1:A:378:LYS:N	2.28	0.66
1:A:169:MET:HE3	1:A:531:ALA:HB2	1.77	0.65
1:A:413:LYS:O	1:A:415:THR:N	2.29	0.65
1:B:121:HIS:HA	1:B:124:LEU:CG	2.27	0.65
1:B:191:ALA:HB2	1:B:198:VAL:HG23	1.79	0.65
1:B:501:MET:O	1:B:502:ILE:HD13	1.96	0.65
1:B:556:GLU:N	1:B:556:GLU:OE2	2.30	0.65
1:A:452:PRO:O	1:A:455:ALA:O	2.16	0.64
1:A:127:TRP:CE3	1:A:127:TRP:O	2.50	0.64
2:C:152:PHE:CE1	2:C:159:ILE:HD12	2.33	0.64
1:A:505:THR:OG1	1:A:506:GLU:O	2.09	0.64
1:B:355:ILE:O	1:B:359:GLN:HG2	1.99	0.63
1:B:570:LEU:HD12	1:B:571:HIS:N	2.14	0.63
2:D:268:VAL:HG12	2:D:269:LEU:HG	1.80	0.63
1:B:131:ASN:HB3	1:B:134:THR:HG22	1.81	0.63
1:B:454:VAL:HG11	1:B:587:VAL:HG11	1.80	0.63
1:A:126:ILE:HG22	1:A:489:HIS:O	1.97	0.63
1:A:443:LEU:HD23	1:A:444:PHE:N	2.14	0.63
1:A:119:LEU:HD12	1:A:120:LEU:HD22	1.80	0.63
1:A:262:LEU:HD22	1:A:349:ILE:CD1	2.29	0.63
1:B:58:LEU:HD23	1:B:104:THR:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HD12	1:B:124:LEU:O	1.99	0.63
1:B:64:ASN:HD21	1:B:67:LEU:HB3	1.64	0.62
1:B:151:ILE:HG21	1:B:241:PHE:CE1	2.31	0.62
1:B:515:ASN:HB3	1:B:574:LEU:HD21	1.82	0.62
2:C:161:ILE:HD11	2:C:195:ILE:O	1.98	0.62
2:C:103:ASN:C	2:C:103:ASN:HD22	2.08	0.62
1:A:304:VAL:HG21	1:A:326:LEU:HD23	1.81	0.61
1:A:159:ILE:HD13	1:A:159:ILE:H	1.65	0.61
1:A:81:PRO:O	1:A:83:THR:HG22	2.01	0.61
1:A:250:ILE:HG13	1:A:260:VAL:HG13	1.82	0.61
1:B:151:ILE:HD13	1:B:241:PHE:CZ	2.36	0.61
1:A:189:ILE:CD1	1:A:502:ILE:HD12	2.17	0.61
1:B:351:ASP:HB3	1:B:356:LEU:CD2	2.30	0.61
1:A:333:PRO:HG3	1:A:339:ALA:HB2	1.81	0.61
1:B:395:PHE:CD1	1:B:440:LEU:HD21	2.36	0.60
1:A:526:TYR:CE2	1:A:570:LEU:HD21	2.37	0.60
1:B:55:ILE:HB	1:B:103:THR:CG2	2.32	0.60
1:A:338:ILE:HD12	1:A:341:GLY:HA3	1.82	0.60
2:D:97:THR:OG1	2:D:244:ILE:HD12	2.01	0.60
2:D:236:ILE:HD12	2:D:236:ILE:O	2.01	0.60
1:A:136:MET:HB3	1:A:139:VAL:CG1	2.32	0.60
1:A:217:ALA:HB2	1:A:312:THR:HG23	1.81	0.60
1:B:132:LEU:O	1:B:135:LEU:HD22	2.01	0.60
1:A:207:ILE:CD1	1:A:300:LEU:HD11	2.31	0.60
1:B:129:THR:O	1:B:130:ALA:HB2	2.02	0.60
1:A:102:ASN:HD22	3:A:1599:NAG:H82	1.67	0.60
1:A:435:THR:O	1:A:439:THR:HG23	2.01	0.60
2:D:172:LYS:HZ2	2:D:173:TYR:H	1.48	0.60
1:A:344:ILE:HD13	1:A:344:ILE:N	2.16	0.59
1:B:74:LEU:HD22	1:B:106:PHE:CE1	2.37	0.59
2:C:168:ILE:C	2:C:168:ILE:HD12	2.27	0.59
1:A:70:VAL:HG21	1:A:188:SER:CB	2.32	0.59
2:D:192:TRP:HB3	2:D:193:PRO:CD	2.32	0.59
1:A:149:LEU:HD13	1:A:151:ILE:HD13	1.83	0.59
2:C:102:PRO:O	2:C:103:ASN:ND2	2.35	0.59
1:A:195:ASN:HD22	1:A:195:ASN:C	2.11	0.59
1:B:55:ILE:HD13	1:B:76:VAL:HG22	1.84	0.59
1:A:422:PHE:HB2	1:B:593:LEU:HD13	1.84	0.59
1:B:335:THR:OG1	1:B:405:ASN:ND2	2.36	0.59
1:B:363:LEU:N	1:B:363:LEU:HD22	2.17	0.59
1:A:593:LEU:HD21	1:B:419:THR:OG1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:OD2	1:A:352:ASP:N	2.27	0.58
1:A:505:THR:HG23	1:A:508:PHE:HB2	1.85	0.58
1:A:377:LEU:HD22	1:A:485:ALA:HB1	1.83	0.58
1:A:135:LEU:N	1:A:135:LEU:HD23	2.18	0.58
2:C:166:ALA:HB3	2:C:192:TRP:CZ3	2.38	0.58
2:C:234:LEU:HD22	2:C:236:ILE:CD1	2.34	0.58
2:D:261:LEU:HD13	2:D:268:VAL:HB	1.84	0.58
2:C:88:ILE:HG13	2:C:288:VAL:HG22	1.86	0.58
1:A:371:VAL:HG21	1:A:450:VAL:HG22	1.85	0.58
2:D:88:ILE:O	2:D:285:VAL:HG13	2.03	0.58
1:A:64:ASN:OD1	1:A:65:GLU:N	2.37	0.58
1:A:410:PRO:O	1:A:412:GLY:N	2.30	0.58
1:B:403:VAL:HG13	1:B:416:LEU:HD23	1.84	0.58
2:D:131:SER:O	2:D:241:ALA:CB	2.51	0.58
1:A:387:GLU:O	1:A:388:ASP:HB2	2.04	0.57
1:A:569:TYR:CZ	1:A:579:ARG:HB2	2.40	0.57
1:B:364:ASN:HD22	1:B:364:ASN:H	1.51	0.57
1:A:207:ILE:CD1	1:A:300:LEU:CD1	2.82	0.57
2:C:154:VAL:HG12	2:C:237:PHE:HA	1.87	0.57
1:B:361:GLU:HG3	2:C:236:ILE:HD11	1.86	0.57
1:A:147:LEU:HD22	1:A:226:ASP:HB3	1.87	0.57
1:B:62:LEU:HD22	1:B:68:GLY:O	2.03	0.57
2:D:269:LEU:HD23	2:D:272:ALA:CB	2.34	0.57
1:A:169:MET:HE3	1:A:531:ALA:HB3	1.86	0.57
1:B:87:ARG:HD3	1:B:144:GLU:OE1	2.04	0.57
1:B:359:GLN:HB3	2:C:234:LEU:HD11	1.86	0.57
1:A:125:PRO:O	1:A:126:ILE:C	2.48	0.57
1:A:134:THR:HG22	1:A:134:THR:O	2.05	0.57
1:B:151:ILE:HD13	1:B:241:PHE:HZ	1.69	0.57
2:D:121:GLN:OE1	2:D:254:PHE:HA	2.05	0.56
1:B:62:LEU:CD2	1:B:68:GLY:O	2.53	0.56
1:A:334:ALA:O	1:A:335:THR:C	2.49	0.56
1:B:144:GLU:OE2	1:B:208:LEU:HD11	2.04	0.56
1:B:234:ILE:HG23	1:B:238:VAL:HB	1.86	0.56
1:A:593:LEU:HD22	1:B:419:THR:HA	1.87	0.56
1:B:127:TRP:CE3	1:B:507:LEU:HD21	2.41	0.56
1:B:304:VAL:HG13	1:B:321:LYS:HE2	1.88	0.56
1:A:70:VAL:HG21	1:A:188:SER:HB2	1.88	0.56
1:B:139:VAL:O	1:B:139:VAL:CG1	2.52	0.56
1:B:48:VAL:HG13	1:B:241:PHE:HB3	1.87	0.56
2:C:113:LEU:HD12	2:C:114:ALA:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:ILE:HD13	2:D:258:LEU:HD22	1.87	0.56
1:A:86:ARG:O	1:A:87:ARG:C	2.48	0.56
1:A:136:MET:HB3	1:A:139:VAL:HG11	1.87	0.55
1:B:250:ILE:HG23	1:B:250:ILE:O	2.06	0.55
1:A:413:LYS:O	1:A:414:ASP:C	2.48	0.55
1:A:322:ASN:C	1:A:324:LYS:N	2.64	0.55
1:B:268:TYR:CD2	1:B:348:VAL:HG23	2.42	0.55
1:A:139:VAL:HG13	1:A:140:GLN:N	2.05	0.55
1:A:407:TYR:HD2	1:A:407:TYR:N	2.05	0.55
2:D:261:LEU:HD23	2:D:262:TYR:H	1.72	0.55
1:A:196:VAL:HG11	1:A:528:THR:HG23	1.88	0.55
1:A:369:LEU:HD23	1:A:369:LEU:H	1.71	0.55
1:A:559:TRP:CE3	1:A:570:LEU:HD23	2.41	0.55
1:A:410:PRO:C	1:A:412:GLY:H	2.15	0.55
2:D:115:ILE:CD1	2:D:258:LEU:HD22	2.36	0.55
1:A:352:ASP:HB3	1:A:355:ILE:HD12	1.89	0.55
1:A:594:VAL:HG12	1:A:595:PRO:HD3	1.88	0.55
1:A:494:PRO:HB3	1:A:499:ILE:HD12	1.89	0.54
1:B:590:TRP:CE3	1:B:594:VAL:HG21	2.42	0.54
1:A:455:ALA:O	1:A:456:THR:HB	2.07	0.54
1:A:476:CYS:O	1:A:477:GLN:O	2.25	0.54
1:A:357:MET:O	1:A:359:GLN:N	2.40	0.54
1:A:395:PHE:CD1	1:A:440:LEU:HD13	2.42	0.54
1:B:502:ILE:HG22	1:B:503:GLY:H	1.73	0.54
2:C:85:THR:HG21	2:C:273:ALA:HB2	1.88	0.54
1:A:488:ALA:N	1:A:491:ASP:OD1	2.41	0.54
1:A:114:LEU:HD22	1:A:114:LEU:N	2.22	0.54
1:B:221:ASN:O	1:B:225:LEU:HD12	2.08	0.54
2:D:88:ILE:HG22	2:D:286:ARG:HB2	1.90	0.54
1:A:273:PHE:CE2	1:A:365:TYR:CE1	2.96	0.54
1:B:139:VAL:O	1:B:142:GLN:NE2	2.41	0.54
1:A:377:LEU:H	1:A:441:VAL:HG13	1.72	0.54
1:A:407:TYR:N	1:A:407:TYR:CD2	2.75	0.54
1:A:583:ARG:O	1:A:584:ALA:C	2.51	0.54
2:D:186:THR:HG23	2:D:194:VAL:CG1	2.38	0.54
1:A:149:LEU:C	1:A:149:LEU:HD12	2.33	0.53
1:A:175:GLY:O	1:A:255:ALA:CB	2.57	0.53
1:A:593:LEU:O	1:A:594:VAL:HG23	2.09	0.53
1:A:277:ILE:HG21	1:A:368:MET:HE2	1.90	0.53
1:B:62:LEU:HD23	1:B:67:LEU:HD13	1.91	0.53
1:B:67:LEU:HD22	1:B:68:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:ASP:HA	2:D:153:ASN:O	2.08	0.53
2:D:261:LEU:HD13	2:D:268:VAL:CG1	2.39	0.53
1:A:131:ASN:O	1:A:133:ASP:N	2.42	0.53
1:A:216:GLN:N	1:A:216:GLN:CD	2.67	0.53
1:A:61:PRO:HA	1:A:69:PRO:HA	1.91	0.53
1:A:102:ASN:HD22	3:A:1599:NAG:C8	2.21	0.53
1:A:451:ALA:HA	1:A:587:VAL:HG13	1.91	0.53
1:B:67:LEU:HD11	1:B:192:SER:OG	2.09	0.53
2:C:115:ILE:HD11	2:C:258:LEU:HB3	1.90	0.53
1:A:594:VAL:HG12	1:A:595:PRO:CD	2.40	0.52
1:B:156:GLU:OE1	1:B:195:ASN:ND2	2.41	0.52
1:B:327:ILE:O	1:B:329:GLN:N	2.41	0.52
1:A:494:PRO:HB3	1:A:508:PHE:CD2	2.44	0.52
1:A:217:ALA:HB2	1:A:312:THR:CG2	2.38	0.52
1:B:115:ASP:O	1:B:116:GLU:C	2.52	0.52
1:B:251:PHE:HB2	1:B:277:ILE:HB	1.91	0.52
1:A:403:VAL:HG21	1:A:417:ARG:HB2	1.91	0.52
1:B:135:LEU:HD22	1:B:136:MET:N	2.24	0.52
1:A:373:GLN:O	1:A:445:THR:HG21	2.10	0.52
1:A:506:GLU:O	1:A:507:LEU:HB2	2.08	0.52
1:A:149:LEU:HD12	1:A:149:LEU:O	2.09	0.52
1:A:82:PRO:HA	1:A:86:ARG:HB2	1.91	0.52
1:B:62:LEU:HD23	1:B:67:LEU:CD1	2.40	0.52
1:B:129:THR:HG21	1:B:378:LYS:CE	2.38	0.52
2:D:115:ILE:HD12	2:D:261:LEU:CD1	2.39	0.52
1:A:395:PHE:CZ	1:A:425:THR:HG23	2.44	0.52
1:B:357:MET:HB3	1:B:459:LEU:HD13	1.92	0.52
1:A:228:ILE:HD12	1:A:228:ILE:N	2.25	0.52
1:A:277:ILE:HA	1:A:368:MET:O	2.10	0.52
1:B:82:PRO:HD2	1:B:145:ASP:HA	1.91	0.52
1:B:211:LEU:HD11	1:B:297:THR:HG23	1.92	0.52
1:B:424:TYR:CE2	1:B:443:LEU:HA	2.45	0.52
2:D:88:ILE:CG2	2:D:286:ARG:HB2	2.40	0.52
1:A:511:ASN:ND2	3:A:1600:NAG:C1	2.73	0.51
1:A:559:TRP:O	1:A:560:SER:CB	2.58	0.51
1:B:525:THR:HG22	1:B:529:ASN:OD1	2.09	0.51
1:B:594:VAL:HG12	1:B:595:PRO:N	2.25	0.51
2:D:115:ILE:HG12	2:D:258:LEU:HD22	1.92	0.51
1:A:402:PHE:CE1	1:A:406:LEU:CD1	2.94	0.51
1:B:131:ASN:O	1:B:134:THR:N	2.43	0.51
1:A:175:GLY:HA3	1:A:179:GLU:OE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:VAL:O	1:A:597:LEU:HG	2.11	0.51
1:B:581:HIS:HB3	1:B:584:ALA:CB	2.40	0.51
2:D:88:ILE:HG23	2:D:89:PHE:N	2.26	0.51
1:B:129:THR:O	1:B:130:ALA:CB	2.58	0.51
1:A:136:MET:C	1:A:139:VAL:HG12	2.36	0.51
1:A:212:SER:CB	1:A:343:VAL:HG21	2.41	0.51
1:B:354:GLN:O	1:B:355:ILE:C	2.54	0.51
2:C:278:ASN:C	2:C:278:ASN:HD22	2.19	0.51
2:D:129:VAL:HG12	2:D:243:ILE:HG12	1.92	0.51
1:A:406:LEU:HD13	1:A:447:HIS:CE1	2.46	0.51
1:B:377:LEU:O	1:B:377:LEU:HD12	2.11	0.51
1:B:409:TYR:HB3	1:B:410:PRO:HD3	1.93	0.51
1:B:410:PRO:O	1:B:411:GLU:C	2.54	0.51
1:A:470:TYR:CD1	1:A:470:TYR:C	2.89	0.51
1:A:234:ILE:O	1:A:235:GLU:C	2.55	0.50
1:B:217:ALA:HB2	1:B:312:THR:HG23	1.92	0.50
1:B:526:TYR:HE2	1:B:570:LEU:HD23	1.76	0.50
2:D:117:PHE:HB3	2:D:258:LEU:HD23	1.93	0.50
1:A:59:ARG:NH1	1:A:155:THR:HG21	2.26	0.50
1:A:364:ASN:ND2	2:D:106:PRO:O	2.44	0.50
1:A:399:VAL:HG21	1:A:421:LYS:HB3	1.92	0.50
2:C:271:MET:HB3	2:C:279:ILE:HD11	1.93	0.50
2:D:119:THR:O	2:D:171:GLY:N	2.44	0.50
2:D:141:LEU:CD1	2:D:148:ILE:HG23	2.30	0.50
1:A:172:ILE:HG21	1:A:259:CYS:HB2	1.93	0.50
1:A:451:ALA:O	1:A:591:LEU:HD11	2.12	0.50
1:B:55:ILE:HG22	1:B:101:ARG:HB3	1.92	0.50
1:B:369:LEU:N	1:B:369:LEU:HD23	2.26	0.50
1:A:367:ILE:O	1:A:367:ILE:HG22	2.10	0.50
1:B:268:TYR:HD2	1:B:348:VAL:HG23	1.77	0.50
2:C:234:LEU:CD2	2:C:236:ILE:CD1	2.90	0.50
1:A:223:GLY:O	1:A:225:LEU:N	2.45	0.50
1:A:132:LEU:C	1:A:132:LEU:HD22	2.37	0.50
2:C:192:TRP:HB3	2:C:193:PRO:CD	2.42	0.50
1:A:495:TYR:CD1	1:A:519:LEU:HD23	2.47	0.50
1:A:563:ASN:N	1:A:563:ASN:OD1	2.43	0.50
1:B:228:ILE:HG23	1:B:272:LEU:CD1	2.42	0.50
2:C:200:ALA:HA	2:C:231:GLY:N	2.27	0.50
1:B:127:TRP:CZ3	1:B:507:LEU:HD21	2.46	0.50
2:D:115:ILE:CG1	2:D:258:LEU:HD22	2.42	0.50
2:D:152:PHE:O	2:D:159:ILE:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:LEU:HD11	2:C:258:LEU:HD21	1.93	0.49
1:A:470:TYR:HB3	1:A:559:TRP:CZ2	2.47	0.49
1:B:168:VAL:CG1	1:B:199:ILE:HD12	2.42	0.49
1:B:364:ASN:HD22	1:B:364:ASN:N	2.10	0.49
2:D:129:VAL:CG2	2:D:139:LEU:HB3	2.42	0.49
2:D:186:THR:HG23	2:D:194:VAL:HG13	1.94	0.49
2:D:126:LEU:CD1	2:D:127:VAL:HG23	2.42	0.49
1:A:282:THR:OG1	1:A:283:ALA:N	2.45	0.49
1:B:119:LEU:C	1:B:120:LEU:HD13	2.37	0.49
1:B:129:THR:O	1:B:129:THR:CG2	2.53	0.49
2:C:234:LEU:HD22	2:C:236:ILE:HD12	1.95	0.49
1:A:234:ILE:HG23	1:A:238:VAL:HB	1.93	0.49
1:A:264:THR:HG22	1:A:365:TYR:CD2	2.47	0.49
1:A:289:VAL:HG23	1:A:291:TYR:HE2	1.77	0.49
1:A:322:ASN:C	1:A:324:LYS:H	2.19	0.49
2:C:161:ILE:HG23	2:C:187:LEU:HD22	1.94	0.49
1:A:368:MET:HE1	1:A:527:TRP:CE3	2.48	0.49
1:B:230:ALA:O	1:B:233:TRP:HB3	2.13	0.49
1:B:300:LEU:O	1:B:300:LEU:HD23	2.12	0.49
1:B:525:THR:O	1:B:529:ASN:ND2	2.46	0.49
1:A:132:LEU:HD22	1:A:132:LEU:O	2.13	0.49
1:A:207:ILE:HG13	1:A:340:PHE:CE1	2.48	0.49
1:A:400:SER:HA	1:A:403:VAL:HG22	1.95	0.49
1:B:493:VAL:N	1:B:494:PRO:HD2	2.28	0.49
2:C:137:ASP:HA	2:C:153:ASN:O	2.13	0.49
1:A:50:THR:N	1:A:53:GLY:O	2.46	0.49
1:B:110:CYS:O	1:B:112:GLN:HG2	2.13	0.49
2:D:96:ILE:CG2	2:D:245:ILE:HB	2.41	0.49
1:A:390:VAL:HG23	1:A:437:ARG:HA	1.94	0.48
2:D:176:VAL:HG22	2:D:189:VAL:HG13	1.96	0.48
1:B:304:VAL:HG13	1:B:321:LYS:CE	2.43	0.48
2:D:117:PHE:HB2	2:D:257:GLN:O	2.13	0.48
2:D:141:LEU:HD11	2:D:148:ILE:HG22	1.92	0.48
2:D:192:TRP:CB	2:D:193:PRO:CD	2.91	0.48
1:A:408:GLY:C	1:A:410:PRO:HD3	2.38	0.48
1:B:451:ALA:HB3	1:B:452:PRO:CD	2.43	0.48
2:C:117:PHE:CE1	2:C:168:ILE:HD13	2.48	0.48
2:D:159:ILE:HG22	2:D:160:ALA:N	2.27	0.48
1:B:431:GLU:O	1:B:432:ASN:C	2.57	0.48
1:A:76:VAL:CG2	1:A:103:THR:HG21	2.44	0.48
1:B:144:GLU:CD	1:B:208:LEU:HD11	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LEU:HD11	1:B:576:PRO:HB2	1.96	0.48
1:A:144:GLU:HG3	1:A:208:LEU:HD11	1.95	0.48
1:B:121:HIS:O	1:B:124:LEU:CD1	2.62	0.48
1:A:280:SER:OG	1:A:375:GLU:OE1	2.32	0.48
1:A:455:ALA:O	1:A:456:THR:CB	2.61	0.48
2:C:179:THR:O	2:C:185:ALA:HB1	2.13	0.48
1:A:443:LEU:O	1:A:444:PHE:C	2.56	0.48
1:A:190:LEU:O	1:A:191:ALA:C	2.56	0.47
1:A:263:LEU:O	1:A:264:THR:C	2.57	0.47
1:B:250:ILE:HD13	1:B:263:LEU:HD11	1.95	0.47
2:D:127:VAL:CG2	2:D:245:ILE:HG23	2.38	0.47
1:B:423:MET:CE	1:B:423:MET:HA	2.44	0.47
1:A:528:THR:O	1:A:531:ALA:N	2.46	0.47
1:B:118:SER:O	1:B:119:LEU:HD22	2.14	0.47
1:B:518:MET:O	1:B:521:ALA:HB3	2.15	0.47
1:A:59:ARG:CZ	1:A:155:THR:HG21	2.44	0.47
1:A:261:SER:O	1:A:264:THR:OG1	2.32	0.47
1:B:436:ARG:O	1:B:440:LEU:HD23	2.14	0.47
2:C:154:VAL:HG12	2:C:237:PHE:CA	2.44	0.47
1:A:304:VAL:HG12	1:A:306:CYS:SG	2.55	0.47
1:B:213:THR:HG21	1:B:311:THR:HB	1.96	0.47
1:A:431:GLU:O	1:A:432:ASN:C	2.58	0.47
1:B:213:THR:HG23	1:B:218:ALA:HB3	1.96	0.47
1:B:250:ILE:CD1	1:B:263:LEU:CD1	2.90	0.47
1:B:348:VAL:HG13	1:B:349:ILE:HG12	1.96	0.47
1:B:403:VAL:HG21	1:B:417:ARG:HA	1.97	0.47
2:C:126:LEU:HD11	2:C:258:LEU:CD2	2.44	0.47
1:A:429:ASP:HB3	1:A:432:ASN:HB3	1.97	0.47
1:B:120:LEU:HD13	1:B:120:LEU:N	2.30	0.47
1:B:189:ILE:HD11	1:B:501:MET:HB2	1.97	0.47
2:C:287:LEU:HD12	2:C:287:LEU:N	2.28	0.47
2:D:130:ASP:O	2:D:131:SER:OG	2.30	0.47
1:A:117:ARG:O	1:A:118:SER:HB3	2.15	0.47
1:A:130:ALA:O	1:A:131:ASN:CB	2.62	0.47
1:B:109:VAL:HG11	1:B:112:GLN:NE2	2.29	0.47
2:D:285:VAL:CG1	2:D:286:ARG:N	2.78	0.47
1:A:529:ASN:HB3	1:A:539:PRO:HD2	1.97	0.47
1:B:248:VAL:HB	1:B:273:PHE:HA	1.97	0.46
1:B:293:PRO:O	1:B:297:THR:N	2.48	0.46
1:B:408:GLY:O	1:B:409:TYR:HB3	2.15	0.46
2:D:247:GLY:HA2	2:D:250:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASN:HD21	3:A:1600:NAG:C6	2.28	0.46
2:D:232:ARG:HD3	2:D:232:ARG:O	2.14	0.46
1:A:374:GLY:O	1:A:488:ALA:HA	2.16	0.46
1:A:559:TRP:O	1:A:560:SER:OG	2.33	0.46
1:B:178:MET:C	1:B:179:GLU:HG3	2.40	0.46
1:B:568:LEU:HD13	1:B:568:LEU:N	2.31	0.46
1:A:125:PRO:O	1:A:127:TRP:N	2.48	0.46
1:A:135:LEU:HD22	1:A:507:LEU:H	1.80	0.46
1:A:443:LEU:O	1:A:446:ASP:N	2.49	0.46
2:C:139:LEU:C	2:C:139:LEU:HD12	2.40	0.46
1:A:424:TYR:CE2	1:A:443:LEU:HA	2.50	0.46
1:A:449:TRP:O	1:A:453:ALA:CB	2.64	0.46
1:B:418:GLU:O	1:B:421:LYS:HB3	2.15	0.46
1:A:207:ILE:HD11	1:A:300:LEU:HD13	1.98	0.46
1:B:109:VAL:HG12	1:B:110:CYS:H	1.81	0.46
1:B:507:LEU:C	1:B:507:LEU:CD2	2.89	0.46
1:B:587:VAL:HG12	1:B:591:LEU:HD12	1.96	0.46
1:B:526:TYR:HE2	1:B:570:LEU:CD2	2.29	0.46
1:B:533:THR:HG21	1:B:538:GLN:C	2.40	0.46
2:D:117:PHE:O	2:D:173:TYR:HA	2.16	0.46
1:A:70:VAL:HG21	1:A:188:SER:HB3	1.98	0.46
1:B:470:TYR:C	1:B:470:TYR:CD1	2.94	0.46
1:A:207:ILE:HA	1:A:340:PHE:CD1	2.51	0.45
1:A:563:ASN:O	1:A:565:LYS:N	2.50	0.45
1:A:594:VAL:HG12	1:A:595:PRO:N	2.30	0.45
2:D:285:VAL:HG12	2:D:286:ARG:N	2.31	0.45
1:A:257:ALA:HB1	1:A:278:ILE:HG23	1.97	0.45
1:A:350:PRO:HD2	1:A:356:LEU:HD11	1.99	0.45
1:A:377:LEU:N	1:A:441:VAL:HG13	2.31	0.45
1:A:392:PRO:C	1:A:394:ASP:H	2.24	0.45
2:D:105:ARG:HH11	2:D:241:ALA:HB1	1.82	0.45
1:B:83:THR:HG23	1:B:84:GLY:N	2.31	0.45
1:B:350:PRO:HG2	1:B:356:LEU:HD11	1.98	0.45
1:B:529:ASN:N	1:B:529:ASN:HD22	2.14	0.45
1:B:566:ASP:HB3	1:B:568:LEU:HD11	1.99	0.45
1:A:80:SER:O	1:A:81:PRO:C	2.59	0.45
2:C:200:ALA:CA	2:C:231:GLY:N	2.80	0.45
1:A:102:ASN:ND2	3:A:1599:NAG:C1	2.79	0.45
1:A:126:ILE:HD13	1:A:127:TRP:N	2.32	0.45
1:A:593:LEU:CD2	1:B:419:THR:HA	2.46	0.45
1:B:287:TRP:HE3	1:B:336:TYR:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:236:ILE:O	2:D:236:ILE:CD1	2.65	0.45
1:A:354:GLN:O	1:A:358:GLU:HB2	2.17	0.45
1:A:501:MET:HE3	1:A:524:MET:CE	2.47	0.45
1:B:149:LEU:O	1:B:149:LEU:HD12	2.16	0.45
1:B:407:TYR:OH	1:B:594:VAL:HG11	2.17	0.45
2:C:102:PRO:O	2:C:103:ASN:CB	2.64	0.45
1:A:262:LEU:HD22	1:A:349:ILE:HD13	1.99	0.45
2:D:124:ALA:HB3	2:D:143:ILE:HB	1.98	0.45
2:D:131:SER:OG	2:D:132:SER:N	2.49	0.45
1:A:149:LEU:CD1	1:A:149:LEU:C	2.90	0.45
1:A:570:LEU:HD12	1:A:571:HIS:H	1.82	0.45
1:B:87:ARG:HG2	1:B:208:LEU:HD21	1.99	0.45
1:B:100:ILE:HG22	1:B:101:ARG:H	1.81	0.45
1:B:368:MET:HE2	1:B:536:PRO:HG3	1.96	0.45
1:A:228:ILE:N	1:A:228:ILE:CD1	2.80	0.45
1:B:189:ILE:HG23	1:B:497:PHE:O	2.16	0.45
1:B:322:ASN:C	1:B:324:LYS:H	2.23	0.45
2:C:200:ALA:C	2:C:231:GLY:N	2.75	0.45
1:A:123:MET:SD	1:A:176:SER:OG	2.73	0.45
1:A:273:PHE:CE2	1:A:365:TYR:CD1	3.05	0.45
1:A:559:TRP:CD2	1:A:570:LEU:HD23	2.52	0.45
1:B:580:ASP:O	1:B:581:HIS:HB2	2.17	0.45
2:C:170:ASP:OD1	2:C:170:ASP:N	2.49	0.45
2:D:194:VAL:HG12	2:D:194:VAL:O	2.17	0.45
1:A:117:ARG:O	1:A:118:SER:CB	2.64	0.44
1:A:424:TYR:CD2	1:A:443:LEU:HB2	2.51	0.44
1:B:67:LEU:HD13	1:B:67:LEU:C	2.42	0.44
1:B:432:ASN:C	1:B:432:ASN:OD1	2.60	0.44
2:D:154:VAL:HG11	2:D:180:ARG:NH1	2.32	0.44
1:A:137:THR:HG22	1:A:137:THR:O	2.16	0.44
1:B:361:GLU:HA	2:C:236:ILE:CG1	2.47	0.44
1:A:184:MET:HB2	1:A:507:LEU:HD21	2.00	0.44
1:A:403:VAL:CG1	1:A:420:ILE:HD12	2.48	0.44
1:B:499:ILE:N	1:B:500:PRO:CD	2.80	0.44
1:B:525:THR:O	1:B:529:ASN:CG	2.59	0.44
2:D:188:GLN:HG3	2:D:194:VAL:HG22	1.99	0.44
1:A:406:LEU:C	1:A:407:TYR:HD2	2.24	0.44
1:B:131:ASN:O	1:B:132:LEU:C	2.60	0.44
2:C:274:GLU:O	2:C:275:ASN:HB3	2.17	0.44
2:D:101:PRO:O	2:D:104:ASP:N	2.50	0.44
2:D:126:LEU:CD2	2:D:143:ILE:HD11	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD12	1:B:119:LEU:HG	1.99	0.44
2:D:108:THR:HG22	2:D:109:ARG:N	2.32	0.44
2:D:115:ILE:HG23	2:D:115:ILE:O	2.16	0.44
1:A:55:ILE:CD1	1:A:76:VAL:HG21	2.47	0.44
1:A:178:MET:O	1:A:179:GLU:HB3	2.18	0.44
1:A:402:PHE:CZ	1:A:406:LEU:HD12	2.53	0.44
1:B:244:ASP:OD1	1:B:245:PRO:HD2	2.18	0.44
1:A:83:THR:O	1:A:85:GLU:N	2.50	0.44
1:A:168:VAL:HG21	1:A:248:VAL:HG22	2.00	0.44
1:B:126:ILE:HD13	1:B:126:ILE:O	2.18	0.44
1:B:590:TRP:CE3	1:B:590:TRP:HA	2.53	0.44
2:D:97:THR:OG1	2:D:244:ILE:CD1	2.65	0.44
1:A:87:ARG:HD2	1:A:144:GLU:OE2	2.18	0.44
1:A:289:VAL:CG2	1:A:291:TYR:HE2	2.30	0.44
1:A:499:ILE:N	1:A:500:PRO:CD	2.81	0.44
2:C:166:ALA:CB	2:C:192:TRP:CZ3	3.01	0.44
1:A:306:CYS:SG	1:A:318:LEU:HD23	2.58	0.43
1:B:422:PHE:CE2	1:B:423:MET:HE3	2.53	0.43
1:B:423:MET:HA	1:B:423:MET:HE2	2.00	0.43
2:D:261:LEU:HD13	2:D:268:VAL:CB	2.47	0.43
1:A:124:LEU:HB3	1:A:125:PRO:CD	2.49	0.43
1:A:139:VAL:CG1	1:A:140:GLN:H	2.08	0.43
1:A:177:TYR:CE2	1:A:338:ILE:HD13	2.53	0.43
1:A:221:ASN:HB3	1:A:224:LEU:CD1	2.48	0.43
1:B:354:GLN:HG2	1:B:358:GLU:OE2	2.18	0.43
2:D:267:LYS:O	2:D:271:MET:HE2	2.18	0.43
1:A:186:ASP:OD1	1:A:186:ASP:C	2.60	0.43
1:A:331:ILE:O	1:A:333:PRO:HD3	2.18	0.43
1:B:61:PRO:HA	1:B:69:PRO:HA	1.98	0.43
1:B:334:ALA:O	1:B:335:THR:C	2.61	0.43
1:B:493:VAL:N	1:B:494:PRO:CD	2.82	0.43
2:C:188:GLN:HB3	2:C:194:VAL:HA	2.00	0.43
2:D:115:ILE:HD12	2:D:261:LEU:HD12	2.00	0.43
1:A:78:TYR:CE2	1:A:230:ALA:HB2	2.53	0.43
1:A:126:ILE:HG23	1:A:127:TRP:H	1.84	0.43
1:A:515:ASN:O	1:A:516:ASP:C	2.62	0.43
1:A:596:HIS:O	1:A:597:LEU:HD23	2.18	0.43
2:C:123:GLU:OE1	2:C:144:HIS:ND1	2.39	0.43
2:D:245:ILE:HD11	2:D:268:VAL:HG11	2.00	0.43
1:A:102:ASN:ND2	3:A:1599:NAG:C2	2.79	0.43
1:A:207:ILE:CD1	1:A:300:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASN:C	1:B:324:LYS:N	2.75	0.43
2:D:117:PHE:CZ	2:D:148:ILE:HG12	2.53	0.43
1:A:361:GLU:OE2	2:D:235:THR:N	2.51	0.43
2:D:244:ILE:O	2:D:244:ILE:HG22	2.18	0.43
1:A:348:VAL:HG12	1:A:349:ILE:N	2.33	0.43
1:A:377:LEU:HD23	1:A:488:ALA:HB2	2.01	0.43
1:A:479:GLU:OE1	1:A:479:GLU:N	2.52	0.43
1:B:299:ILE:CG2	1:B:331:ILE:HG23	2.48	0.43
1:B:375:GLU:OE1	1:B:489:HIS:ND1	2.44	0.43
2:D:135:LEU:HD23	2:D:135:LEU:HA	1.80	0.43
1:A:249:THR:HG23	1:A:275:LYS:O	2.18	0.43
1:B:250:ILE:HD13	1:B:263:LEU:CD1	2.48	0.43
1:B:449:TRP:O	1:B:453:ALA:CB	2.67	0.43
2:C:96:ILE:HG12	2:C:281:ILE:HG23	2.01	0.43
1:A:328:GLN:O	1:A:328:GLN:HG3	2.19	0.43
1:A:570:LEU:HD12	1:A:571:HIS:N	2.34	0.43
2:C:170:ASP:C	2:C:172:LYS:H	2.27	0.43
2:D:129:VAL:HG23	2:D:139:LEU:HB3	1.99	0.43
2:D:198:TYR:O	2:D:199:PRO:C	2.62	0.43
1:A:333:PRO:HG3	1:A:339:ALA:CB	2.49	0.42
1:B:83:THR:O	1:B:86:ARG:N	2.51	0.42
1:B:109:VAL:HG13	1:B:181:THR:HB	2.00	0.42
1:B:317:CYS:O	1:B:320:ASN:HB2	2.19	0.42
1:B:390:VAL:HG23	1:B:437:ARG:HG3	2.01	0.42
2:C:108:THR:HB	2:C:110:ALA:O	2.19	0.42
1:B:83:THR:O	1:B:87:ARG:N	2.51	0.42
1:B:178:MET:HE1	1:B:207:ILE:HG13	2.00	0.42
2:C:85:THR:HG21	2:C:273:ALA:CB	2.48	0.42
1:B:345:ASP:OD2	1:B:348:VAL:HG12	2.18	0.42
2:C:106:PRO:HG2	2:C:240:GLN:HB2	2.02	0.42
2:C:131:SER:HA	2:C:239:SER:O	2.19	0.42
1:A:296:TYR:CD2	1:A:339:ALA:HA	2.54	0.42
1:A:440:LEU:HD12	1:A:440:LEU:HA	1.89	0.42
1:B:315:VAL:HG11	1:B:319:ARG:HH21	1.85	0.42
1:B:372:ASN:OD1	1:B:472:PHE:HB3	2.20	0.42
1:A:60:THR:HB	1:A:72:GLN:NE2	2.34	0.42
1:A:207:ILE:HD13	1:A:326:LEU:O	2.20	0.42
1:A:470:TYR:CD1	1:A:470:TYR:O	2.73	0.42
1:A:533:THR:HG23	1:A:539:PRO:HG3	2.01	0.42
1:B:88:PHE:CE1	1:B:211:LEU:HD23	2.54	0.42
1:B:109:VAL:HG11	1:B:112:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:HIS:O	1:B:124:LEU:HD12	2.19	0.42
1:B:583:ARG:O	1:B:587:VAL:HG23	2.19	0.42
2:D:150:VAL:HG21	2:D:178:PHE:CE1	2.54	0.42
1:A:87:ARG:HD3	1:A:144:GLU:CD	2.45	0.42
1:A:186:ASP:OD1	1:A:188:SER:OG	2.36	0.42
1:A:361:GLU:OE2	2:D:234:LEU:HB3	2.19	0.42
1:B:191:ALA:HB2	1:B:198:VAL:CG2	2.48	0.42
1:A:207:ILE:HG23	1:A:208:LEU:N	2.34	0.42
1:A:443:LEU:HD23	1:A:444:PHE:CA	2.49	0.42
1:B:131:ASN:HB3	1:B:134:THR:CG2	2.49	0.42
1:B:149:LEU:CD1	1:B:151:ILE:HD11	2.49	0.42
1:B:357:MET:C	1:B:459:LEU:HD13	2.44	0.42
1:B:361:GLU:CG	2:C:236:ILE:HD11	2.49	0.42
2:D:96:ILE:HG22	2:D:245:ILE:CB	2.45	0.42
2:D:153:ASN:ND2	2:D:157:ASP:O	2.50	0.42
1:A:409:TYR:N	1:A:410:PRO:CD	2.82	0.42
1:B:89:GLN:HE21	1:B:89:GLN:HA	1.84	0.42
1:B:285:SER:C	1:B:287:TRP:H	2.28	0.42
2:C:86:THR:HG21	2:C:257:GLN:OE1	2.19	0.42
1:A:249:THR:HA	1:A:275:LYS:O	2.19	0.42
1:A:363:LEU:HD23	1:A:365:TYR:OH	2.20	0.42
1:A:418:GLU:O	1:B:593:LEU:HD11	2.20	0.42
1:B:178:MET:HB2	1:B:179:GLU:HG3	2.02	0.42
2:C:103:ASN:C	2:C:103:ASN:ND2	2.76	0.42
2:D:126:LEU:HB2	2:D:143:ILE:HD11	2.02	0.42
2:D:126:LEU:HD12	2:D:127:VAL:HG23	2.01	0.42
2:D:192:TRP:HB3	2:D:193:PRO:HD2	2.00	0.42
1:A:131:ASN:CB	1:A:135:LEU:HD11	2.46	0.41
1:A:359:GLN:O	1:A:463:TYR:CZ	2.73	0.41
1:B:180:GLY:O	1:B:205:LEU:HD11	2.20	0.41
1:B:322:ASN:HB2	1:B:323:TYR:CD1	2.55	0.41
1:B:361:GLU:CA	2:C:236:ILE:HD13	2.41	0.41
1:B:446:ASP:HA	1:B:450:VAL:HB	2.02	0.41
1:B:197:ILE:HD11	1:B:242:GLY:HA3	2.02	0.41
2:C:117:PHE:CD1	2:C:117:PHE:C	2.97	0.41
2:C:265:GLY:C	2:C:266:LEU:HD12	2.45	0.41
1:A:168:VAL:CG2	1:A:248:VAL:HG22	2.50	0.41
1:B:175:GLY:H	1:B:255:ALA:HB3	1.85	0.41
2:C:105:ARG:NH1	2:C:241:ALA:HB1	2.35	0.41
1:A:422:PHE:CG	1:B:593:LEU:HD22	2.56	0.41
1:A:132:LEU:O	1:A:133:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASP:O	1:A:217:ALA:N	2.53	0.41
1:A:511:ASN:ND2	3:A:1600:NAG:O6	2.51	0.41
1:B:465:SER:HA	1:B:466:PRO:HD3	1.96	0.41
2:C:274:GLU:O	2:C:275:ASN:CB	2.67	0.41
2:D:148:ILE:HD13	2:D:168:ILE:CD1	2.49	0.41
1:A:228:ILE:HD11	1:A:263:LEU:HD21	2.01	0.41
1:A:506:GLU:O	1:A:508:PHE:N	2.52	0.41
1:A:136:MET:HB3	1:A:139:VAL:HG12	2.02	0.41
1:A:303:LYS:O	1:A:304:VAL:HG23	2.21	0.41
2:C:192:TRP:CD1	2:C:192:TRP:N	2.86	0.41
2:D:108:THR:HG22	2:D:110:ALA:H	1.86	0.41
1:A:254:GLY:O	1:A:257:ALA:HB3	2.21	0.41
1:B:114:LEU:HA	1:B:119:LEU:HD21	2.02	0.41
1:B:116:GLU:O	1:B:117:ARG:C	2.62	0.41
1:B:132:LEU:HA	1:B:135:LEU:HD11	2.03	0.41
1:B:213:THR:H	1:B:218:ALA:HB3	1.85	0.41
1:B:360:GLY:CA	2:C:238:ASN:HD21	2.34	0.41
1:B:361:GLU:HB2	2:C:234:LEU:HD21	2.02	0.41
2:C:113:LEU:O	2:C:178:PHE:N	2.53	0.41
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.78	0.41
1:B:55:ILE:HD13	1:B:76:VAL:CG2	2.48	0.41
1:B:369:LEU:N	1:B:369:LEU:CD2	2.84	0.41
1:B:374:GLY:O	1:B:488:ALA:HA	2.20	0.41
1:B:566:ASP:HB3	1:B:568:LEU:CD1	2.50	0.41
1:A:130:ALA:O	1:A:131:ASN:HB3	2.21	0.41
1:A:158:ASP:O	1:A:160:HIS:N	2.53	0.41
1:B:124:LEU:HD12	1:B:124:LEU:C	2.46	0.41
1:B:451:ALA:HB3	1:B:452:PRO:HD3	2.03	0.41
2:C:141:LEU:HD11	2:C:148:ILE:HD11	2.03	0.41
1:A:126:ILE:HG23	1:A:127:TRP:N	2.36	0.40
1:B:69:PRO:O	1:B:155:THR:HG23	2.21	0.40
1:B:120:LEU:HD21	1:B:176:SER:OG	2.20	0.40
1:B:289:VAL:HG11	1:B:291:TYR:CE2	2.55	0.40
1:A:126:ILE:C	1:A:126:ILE:HD13	2.46	0.40
1:A:377:LEU:H	1:A:441:VAL:CG1	2.34	0.40
1:A:463:TYR:CE1	2:D:135:LEU:HD21	2.56	0.40
1:A:566:ASP:HB3	1:A:568:LEU:HD12	2.03	0.40
1:A:361:GLU:HG2	2:D:236:ILE:HD11	2.03	0.40
1:A:410:PRO:C	1:A:412:GLY:N	2.77	0.40
1:A:447:HIS:O	1:A:447:HIS:CG	2.75	0.40
1:A:528:THR:HG22	1:A:532:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ASN:N	1:A:529:ASN:HD22	2.19	0.40
1:B:83:THR:HB	1:B:86:ARG:HG3	2.04	0.40
1:B:368:MET:HE3	1:B:536:PRO:HG3	1.99	0.40
2:C:139:LEU:HB2	2:C:152:PHE:HB3	2.02	0.40
2:D:126:LEU:HD11	2:D:258:LEU:HD21	2.02	0.40
2:D:236:ILE:C	2:D:237:PHE:O	2.64	0.40
1:A:62:LEU:HD12	1:A:62:LEU:HA	1.89	0.40
1:A:499:ILE:C	1:A:501:MET:H	2.28	0.40
2:C:282:VAL:HG22	2:C:283:GLY:N	2.36	0.40
1:A:45:TYR:HB3	1:A:57:GLY:O	2.22	0.40
1:A:582:TYR:CZ	1:A:583:ARG:HD2	2.57	0.40
1:B:123:MET:HE3	1:B:123:MET:HB2	1.98	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	539/588 (92%)	388 (72%)	105 (20%)	46 (8%)	0	10
1	B	540/588 (92%)	419 (78%)	81 (15%)	40 (7%)	1	12
2	C	173/179 (97%)	142 (82%)	28 (16%)	3 (2%)	7	35
2	D	173/179 (97%)	125 (72%)	41 (24%)	7 (4%)	2	21
All	All	1425/1534 (93%)	1074 (75%)	255 (18%)	96 (7%)	1	14

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLY
1	A	87	ARG
1	A	118	SER

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Mol	Chain	Res	Type
1	A	121	HIS
1	A	126	ILE
1	A	132	LEU
1	A	133	ASP
1	A	139	VAL
1	A	304	VAL
1	A	325	GLU
1	A	377	LEU
1	A	388	ASP
1	A	409	TYR
1	A	411	GLU
1	A	413	LYS
1	A	414	ASP
1	A	477	GLN
1	A	481	LYS
1	A	504	PRO
1	A	560	SER
1	A	564	PRO
1	B	111	PRO
1	B	130	ALA
1	B	323	TYR
1	B	361	GLU
1	B	364	ASN
1	B	409	TYR
1	B	413	LYS
1	B	476	CYS
1	B	477	GLN
1	B	556	GLU
1	B	557	VAL
1	B	597	LEU
2	C	275	ASN
2	D	192	TRP
1	A	128	PHE
1	A	141	ASP
1	A	224	LEU
1	A	225	LEU
1	A	358	GLU
1	A	480	MET
1	A	559	TRP
1	A	594	VAL
1	B	66	ILE
1	B	108	ALA

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Mol	Chain	Res	Type
1	B	120	LEU
1	B	155	THR
1	B	156	GLU
1	B	165	LYS
1	B	286	SER
1	B	304	VAL
1	B	321	LYS
1	B	328	GLN
1	B	411	GLU
1	B	412	GLY
1	B	487	SER
1	B	507	LEU
1	B	581	HIS
2	C	103	ASN
2	D	237	PHE
1	A	93	PRO
1	A	145	ASP
1	A	242	GLY
1	A	584	ALA
1	B	176	SER
1	B	182	GLY
1	B	377	LEU
1	B	407	TYR
1	B	410	PRO
1	B	506	GLU
1	A	116	GLU
1	A	216	GLN
1	A	323	TYR
1	A	363	LEU
1	A	366	ASP
1	A	432	ASN
1	B	98	THR
2	C	111	ASP
2	D	131	SER
1	A	443	LEU
1	B	116	GLU
1	B	181	THR
2	D	107	SER
2	D	118	SER
1	A	223	GLY
1	A	235	GLU
1	B	509	SER

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Mol	Chain	Res	Type
2	D	143	ILE
2	D	155	GLY
1	B	209	GLY
1	B	380	VAL
1	B	502	ILE
1	A	125	PRO
1	A	159	ILE
1	A	380	VAL
1	A	254	GLY

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	467/510 (92%)	390 (84%)	77 (16%)	2	13
1	B	466/510 (91%)	396 (85%)	70 (15%)	3	16
2	C	143/143 (100%)	120 (84%)	23 (16%)	2	14
2	D	143/143 (100%)	128 (90%)	15 (10%)	6	25
All	All	1219/1306 (93%)	1034 (85%)	185 (15%)	3	16

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	45	TYR
1	A	47	VAL
1	A	62	LEU
1	A	76	VAL
1	A	80	SER
1	A	87	ARG
1	A	89	GLN
1	A	98	THR
1	A	100	ILE
1	A	105	GLN
1	A	109	VAL

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Mol	Chain	Res	Type
1	A	114	LEU
1	A	119	LEU
1	A	120	LEU
1	A	126	ILE
1	A	129	THR
1	A	132	LEU
1	A	135	LEU
1	A	138	TYR
1	A	149	LEU
1	A	159	ILE
1	A	168	VAL
1	A	179	GLU
1	A	195	ASN
1	A	200	THR
1	A	208	LEU
1	A	211	LEU
1	A	224	LEU
1	A	225	LEU
1	A	226	ASP
1	A	246	LYS
1	A	263	LEU
1	A	282	THR
1	A	289	VAL
1	A	304	VAL
1	A	308	MET
1	A	309	LEU
1	A	311	THR
1	A	312	THR
1	A	322	ASN
1	A	330	THR
1	A	332	THR
1	A	338	ILE
1	A	344	ILE
1	A	348	VAL
1	A	349	ILE
1	A	359	GLN
1	A	364	ASN
1	A	366	ASP
1	A	367	ILE
1	A	390	VAL
1	A	394	ASP
1	A	407	TYR

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Mol	Chain	Res	Type
1	A	415	THR
1	A	425	THR
1	A	436	ARG
1	A	440	LEU
1	A	443	LEU
1	A	477	GLN
1	A	480	MET
1	A	481	LYS
1	A	496	VAL
1	A	502	ILE
1	A	505	THR
1	A	506	GLU
1	A	509	SER
1	A	514	LYS
1	A	529	ASN
1	A	561	ARG
1	A	574	LEU
1	A	575	LYS
1	A	577	ARG
1	A	585	THR
1	A	586	LYS
1	A	594	VAL
1	A	597	LEU
1	B	45	TYR
1	B	62	LEU
1	B	66	ILE
1	B	83	THR
1	B	86	ARG
1	B	92	GLU
1	B	100	ILE
1	B	103	THR
1	B	109	VAL
1	B	113	HIS
1	B	114	LEU
1	B	116	GLU
1	B	120	LEU
1	B	121	HIS
1	B	124	LEU
1	B	126	ILE
1	B	133	ASP
1	B	135	LEU
1	B	140	GLN

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Mol	Chain	Res	Type
1	B	141	ASP
1	B	142	GLN
1	B	145	ASP
1	B	159	ILE
1	B	166	LYS
1	B	170	VAL
1	B	188	SER
1	B	190	LEU
1	B	200	THR
1	B	208	LEU
1	B	216	GLN
1	B	219	LYS
1	B	258	SER
1	B	263	LEU
1	B	266	SER
1	B	267	HIS
1	B	282	THR
1	B	285	SER
1	B	286	SER
1	B	304	VAL
1	B	308	MET
1	B	311	THR
1	B	325	GLU
1	B	332	THR
1	B	356	LEU
1	B	363	LEU
1	B	364	ASN
1	B	367	ILE
1	B	368	MET
1	B	369	LEU
1	B	381	ASP
1	B	386	ASN
1	B	413	LYS
1	B	423	MET
1	B	425	THR
1	B	430	LYS
1	B	439	THR
1	B	454	VAL
1	B	460	HIS
1	B	478	SER
1	B	480	MET
1	B	506	GLU

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Mol	Chain	Res	Type
1	B	557	VAL
1	B	560	SER
1	B	568	LEU
1	B	574	LEU
1	B	577	ARG
1	B	578	VAL
1	B	585	THR
1	B	594	VAL
1	B	597	LEU
2	C	85	THR
2	C	100	TRP
2	C	103	ASN
2	C	108	THR
2	C	122	LYS
2	C	126	LEU
2	C	139	LEU
2	C	142	HIS
2	C	154	VAL
2	C	157	ASP
2	C	159	ILE
2	C	179	THR
2	C	186	THR
2	C	187	LEU
2	C	188	GLN
2	C	234	LEU
2	C	236	ILE
2	C	248	LYS
2	C	271	MET
2	C	278	ASN
2	C	281	ILE
2	C	286	ARG
2	C	287	LEU
2	D	88	ILE
2	D	97	THR
2	D	99	LYS
2	D	100	TRP
2	D	103	ASN
2	D	107	SER
2	D	112	ARG
2	D	118	SER
2	D	130	ASP
2	D	156	THR

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Mol	Chain	Res	Type
2	D	172	LYS
2	D	179	THR
2	D	195	ILE
2	D	236	ILE
2	D	254	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	131	ASN
1	A	195	ASN
1	A	202	ASN
1	A	329	GLN
1	A	364	ASN
1	A	432	ASN
1	A	460	HIS
1	A	489	HIS
1	A	511	ASN
1	A	529	ASN
1	B	51	ASN
1	B	64	ASN
1	B	72	GLN
1	B	89	GLN
1	B	112	GLN
1	B	142	GLN
1	B	143	ASN
1	B	195	ASN
1	B	237	ASN
1	B	307	ASN
1	B	364	ASN
1	B	386	ASN
1	B	405	ASN
1	B	448	GLN
1	B	599	ASN
2	C	103	ASN
2	C	145	GLN
2	C	238	ASN
2	C	252	GLN
2	C	264	ASN
2	C	270	ASN
2	C	275	ASN

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Mol	Chain	Res	Type
2	C	278	ASN
2	D	95	GLN
2	D	103	ASN
2	D	145	GLN
2	D	165	ASN
2	D	188	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	NAG	A	1599	-	14,14,15	0.40	0	17,19,21	1.09	0
3	NAG	A	1600	-	14,14,15	0.34	0	17,19,21	1.09	1 (5%)

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
3	NAG	A	1599	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1600	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1600	NAG	C1-C2-N2	-2.86	105.93	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1599	NAG	C8-C7-N2-C2
3	A	1599	NAG	O7-C7-N2-C2
3	A	1600	NAG	C8-C7-N2-C2
3	A	1600	NAG	O7-C7-N2-C2
3	A	1599	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1599	NAG	5	0
3	A	1600	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	200:ALA	C	231:GLY	N	2.80
1	C	200:ALA	C	231:GLY	N	2.75

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	545/588 (92%)	-0.59	1 (0%) 91 81	50, 72, 77, 86	0
1	B	544/588 (92%)	-0.45	0 100 100	63, 73, 78, 84	0
2	C	177/179 (98%)	-0.72	0 100 100	59, 72, 80, 83	0
2	D	177/179 (98%)	-0.25	3 (1%) 69 48	61, 76, 84, 86	0
All	All	1443/1534 (94%)	-0.52	4 (0%) 90 78	50, 73, 80, 86	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	176	VAL	3.3
2	D	89	PHE	3.0
1	A	597	LEU	2.4
2	D	94	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
3	NAG	A	1599	14/15	0.84	0.06	221,222,224,225	0
3	NAG	A	1600	14/15	0.88	0.07	191,192,193,193	0
4	CA	C	1289	1/1	0.98	0.04	109,109,109,109	0
4	CA	D	1289	1/1	0.99	0.04	134,134,134,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.