



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:42 PM UTC

PDB ID : 3IB9 / pdb_00003ib9
Title : Propionyl-CoA Carboxylase Beta Subunit, D422L
Authors : Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Pham, H.; Melgar, M.M.
Deposited on : 2009-07-15
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<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

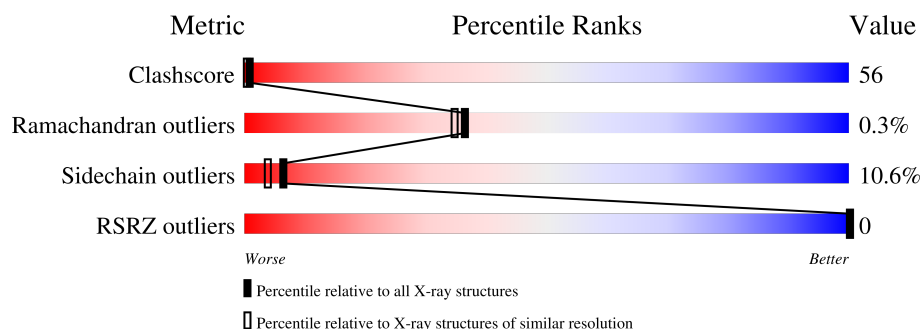
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	530	
1	B	530	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8285 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.

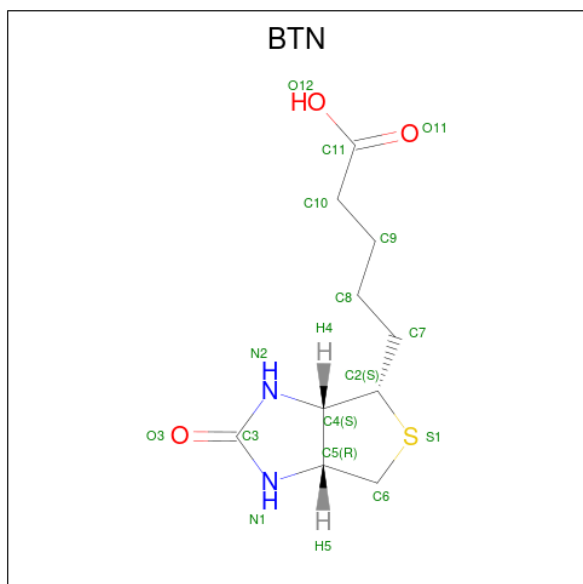
- Molecule 1 is a protein called Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			3952	2483	698	758	13			
1	B	521	Total	C	N	O	S	0	0	0
			3952	2483	698	758	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	LEU	ASP	engineered mutation	UNP Q9X4K7
B	422	LEU	ASP	engineered mutation	UNP Q9X4K7

- Molecule 2 is BIOTIN (CCD ID: BTN) (formula: C₁₀H₁₆N₂O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

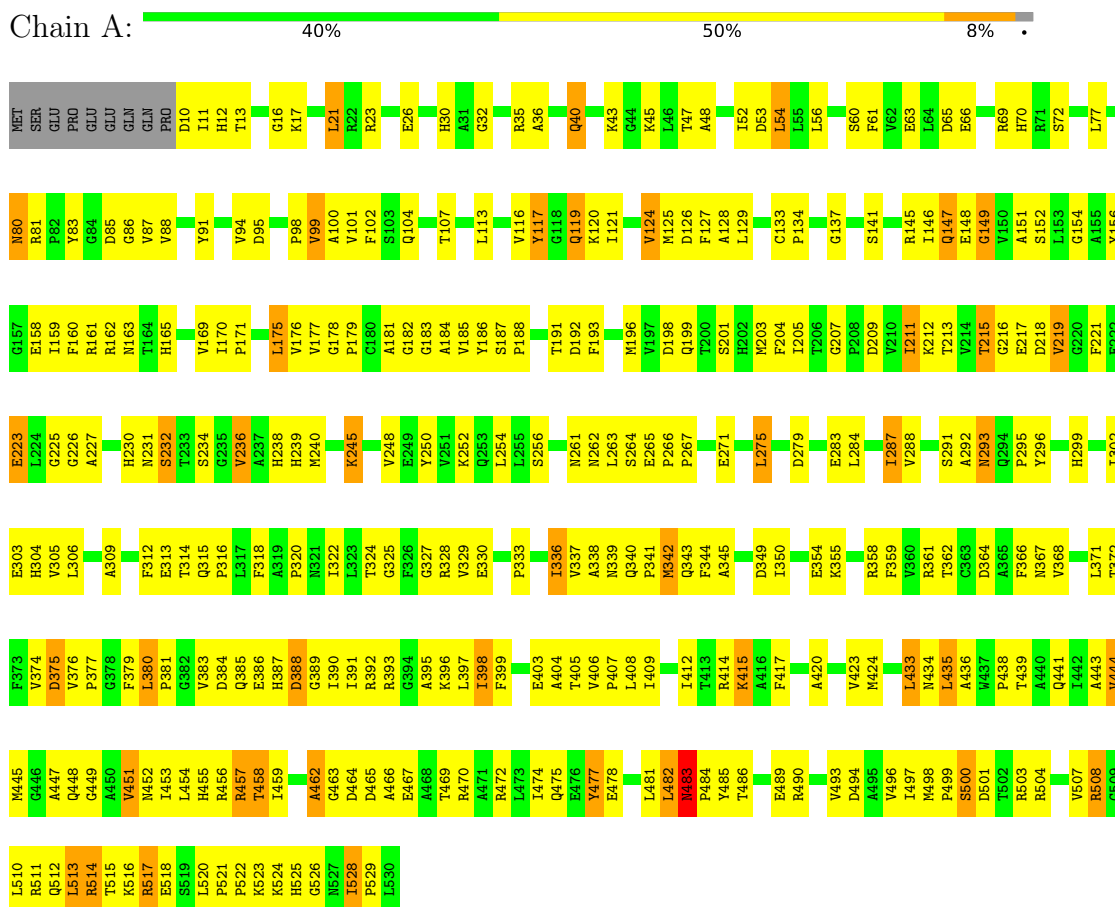
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	172	Total	O	0	0
			172	172		

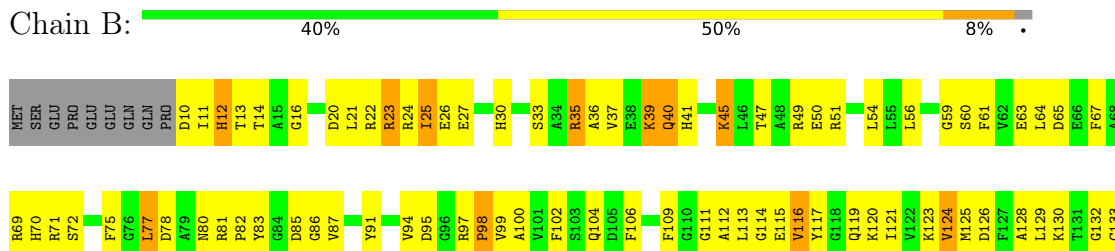
3 Residue-property plots

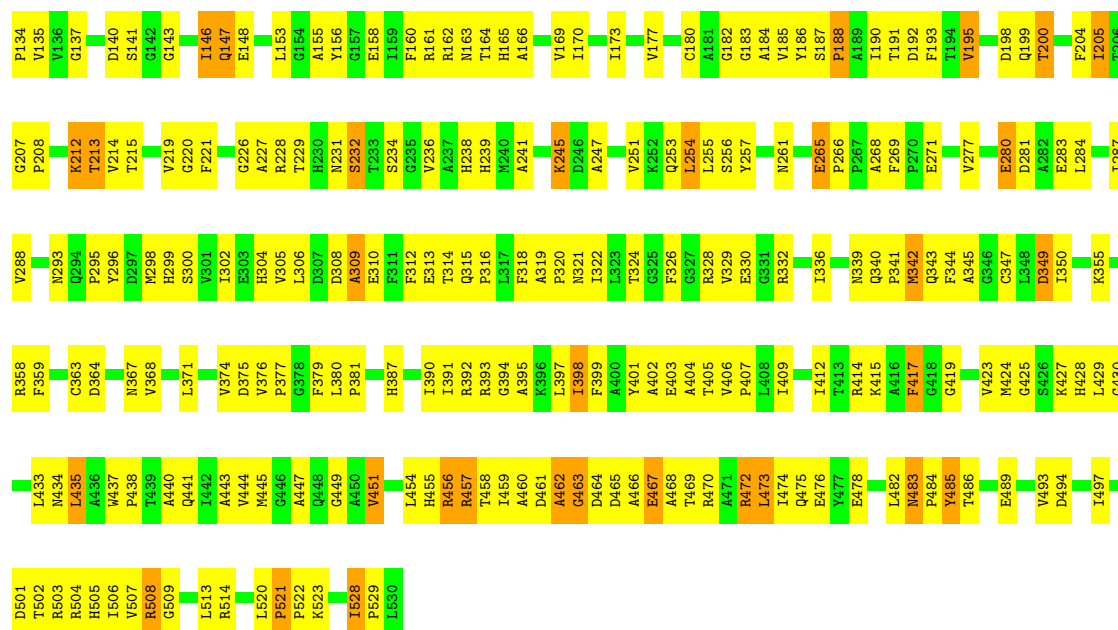
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Propionyl-CoA carboxylase complex B subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	168.49Å 168.49Å 80.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	75.7 (50.00-2.00) 75.7 (50.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-3.70 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.274 0.315 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8285	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.06% 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: BTN, SO4

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	0.32	0/4032	0.82	11/5478 (0.2%)
1	B	0.34	1/4032 (0.0%)	0.85	14/5478 (0.3%)
All	All	0.33	1/8064 (0.0%)	0.84	25/10956 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	ALA	C-N	5.44	1.40	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	VAL	N-CA-C	10.81	120.69	110.53
1	B	463	GLY	N-CA-C	-7.95	105.57	114.40
1	B	12	HIS	CA-C-N	7.64	133.27	122.72
1	B	12	HIS	C-N-CA	7.64	133.27	122.72
1	A	388	ASP	N-CA-C	-7.43	103.17	111.71
1	B	467	GLU	N-CA-C	-7.03	103.81	112.38
1	A	462	ALA	N-CA-C	6.64	120.24	111.28
1	B	485	TYR	N-CA-C	6.52	121.36	113.41
1	B	188	PRO	CB-CA-C	-6.51	102.17	111.68
1	B	521	PRO	O-C-N	6.00	124.07	121.31
1	B	486	THR	N-CA-C	5.86	117.47	111.14
1	B	116	VAL	CA-C-N	5.70	132.43	121.54
1	B	116	VAL	C-N-CA	5.70	132.43	121.54
1	B	116	VAL	N-CA-C	5.64	115.84	110.42
1	B	462	ALA	N-CA-C	5.39	117.76	111.02
1	A	149	GLY	N-CA-C	5.28	125.69	113.18
1	A	451	VAL	N-CA-C	-5.20	105.32	110.62
1	B	417	PHE	N-CA-C	5.20	117.37	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	TYR	N-CA-C	-5.18	105.54	111.14
1	A	483	ASN	CA-C-N	5.17	124.97	119.28
1	A	483	ASN	C-N-CA	5.17	124.97	119.28
1	B	309	ALA	N-CA-C	-5.17	105.08	111.90
1	A	477	TYR	CB-CA-C	5.11	118.98	110.90
1	A	375	ASP	N-CA-C	-5.06	99.86	108.26
1	A	293	ASN	N-CA-C	5.05	116.86	111.36

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	3952	0	3887	482	0
1	B	3952	0	3887	449	0
2	A	16	0	15	2	0
2	B	16	0	15	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	167	0	0	10	0
4	B	172	0	0	13	0
All	All	8285	0	7804	878	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 56.

All (878) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HB	1:A:117:TYR:CE2	1.33	1.57
1:A:456:ARG:NH1	1:A:457:ARG:HH22	1.30	1.29
1:A:87:VAL:HB	1:A:117:TYR:CD2	1.68	1.26
1:B:113:LEU:HD13	1:B:156:TYR:CE1	1.72	1.25
1:A:456:ARG:NH1	1:A:457:ARG:NH2	1.91	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HD3	1:A:218:ASP:OD1	1.40	1.18
1:A:397:LEU:HD23	1:A:423:VAL:CG1	1.73	1.17
1:B:113:LEU:HD22	1:B:156:TYR:CE1	1.81	1.15
1:A:87:VAL:CB	1:A:117:TYR:CE2	2.30	1.15
1:B:113:LEU:CD1	1:B:156:TYR:HE1	1.62	1.13
1:A:362:THR:O	1:A:366:PHE:HD2	1.33	1.11
1:B:21:LEU:O	1:B:25:ILE:HG22	1.50	1.11
1:B:193:PHE:HA	1:B:238:HIS:CE1	1.87	1.10
1:B:457:ARG:HH11	1:B:457:ARG:CG	1.65	1.10
1:B:397:LEU:HD23	1:B:423:VAL:CG1	1.82	1.09
1:A:187:SER:HB3	1:A:188:PRO:HD3	1.34	1.09
1:A:146:ILE:HG22	1:B:454:LEU:HD11	1.35	1.08
1:A:203:MET:HB2	1:A:230:HIS:NE2	1.68	1.08
1:A:160:PHE:HE1	1:A:187:SER:HB2	1.18	1.08
1:B:113:LEU:HB3	1:B:156:TYR:OH	1.53	1.08
1:A:104:GLN:HG2	1:A:117:TYR:OH	1.54	1.07
1:A:478:GLU:HA	1:A:482:LEU:CD1	1.84	1.07
1:B:349:ASP:CB	1:B:380:LEU:HD12	1.85	1.07
1:A:390:ILE:HG21	1:B:205:ILE:HD11	1.12	1.07
1:A:478:GLU:CA	1:A:482:LEU:HD13	1.85	1.07
1:A:87:VAL:CB	1:A:117:TYR:CD2	2.38	1.05
1:B:392:ARG:HG3	1:B:393:ARG:HG3	1.39	1.05
1:A:146:ILE:CG2	1:B:454:LEU:HD11	1.86	1.04
1:B:113:LEU:HD13	1:B:156:TYR:HE1	0.89	1.04
1:A:478:GLU:HA	1:A:482:LEU:HD13	1.04	1.03
1:A:87:VAL:HB	1:A:117:TYR:HE2	1.21	1.02
1:B:397:LEU:HD23	1:B:423:VAL:HG11	1.39	1.02
1:B:457:ARG:HH11	1:B:457:ARG:HG2	0.88	1.02
1:A:196:MET:SD	1:A:203:MET:HE2	2.02	1.00
1:B:509:GLY:O	1:B:513:LEU:HG	1.60	1.00
1:A:215:THR:HG21	4:A:575:HOH:O	1.62	0.99
1:B:347:CYS:SG	1:B:377:PRO:HG2	2.01	0.99
1:A:397:LEU:HD23	1:A:423:VAL:HG11	1.44	0.99
1:A:160:PHE:CE1	1:A:187:SER:HB2	1.98	0.98
1:A:32:GLY:HA3	1:A:107:THR:HG21	1.43	0.98
1:B:349:ASP:HB2	1:B:380:LEU:HD12	1.42	0.98
1:B:445:MET:HE2	1:B:449:GLY:C	1.87	0.98
1:A:10:ASP:O	1:A:16:GLY:HA3	1.63	0.97
1:A:32:GLY:HA3	1:A:107:THR:CG2	1.94	0.97
1:A:395:ALA:O	1:A:398:ILE:HG23	1.63	0.96
1:A:113:LEU:HD12	1:A:117:TYR:HD1	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:HB	1:B:117:TYR:CE2	2.00	0.96
1:B:257:TYR:CE1	1:B:328:ARG:NH1	2.34	0.95
1:B:98:PRO:O	1:B:99:VAL:HG23	1.67	0.94
1:A:231:ASN:OD1	1:A:240:MET:HB2	1.66	0.94
1:A:405:THR:HG21	1:A:518:GLU:O	1.66	0.94
1:B:326:PHE:HE1	1:B:363:CYS:HG	0.94	0.94
1:A:377:PRO:HG3	1:A:415:LYS:HD3	1.50	0.93
1:A:392:ARG:HG3	1:A:393:ARG:HG3	1.48	0.93
1:A:390:ILE:HG21	1:B:205:ILE:CD1	1.96	0.93
1:A:99:VAL:HG22	1:A:134:PRO:HB2	1.50	0.93
1:B:470:ARG:O	1:B:474:ILE:HG13	1.69	0.93
1:B:198:ASP:OD1	1:B:199:GLN:HG2	1.67	0.93
1:A:362:THR:O	1:A:366:PHE:CD2	2.22	0.92
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.51	0.92
1:A:193:PHE:HA	1:A:238:HIS:CE1	2.04	0.92
1:A:483:ASN:HB2	1:A:484:PRO:HD2	1.50	0.92
1:A:451:VAL:HG21	1:A:474:ILE:HG12	1.51	0.91
1:B:440:ALA:O	1:B:484:PRO:HD3	1.71	0.91
1:B:200:THR:HG23	1:B:200:THR:O	1.70	0.91
1:B:113:LEU:CD2	1:B:156:TYR:CE1	2.54	0.91
1:A:380:LEU:HD22	1:A:381:PRO:HD2	1.49	0.90
1:A:467:GLU:HG3	1:A:470:ARG:HH21	1.34	0.90
1:B:457:ARG:HG2	1:B:457:ARG:NH1	1.62	0.90
1:A:87:VAL:CG1	1:A:117:TYR:CD2	2.54	0.90
1:B:241:ALA:HB3	1:B:247:ALA:HB2	1.53	0.89
1:B:339:ASN:OD1	1:B:424:MET:HE2	1.71	0.89
1:A:457:ARG:HH11	1:A:457:ARG:CG	1.85	0.88
1:B:409:ILE:HD11	1:B:513:LEU:HD12	1.54	0.88
1:B:163:ASN:HB3	1:B:190:ILE:HG21	1.55	0.88
1:B:315:GLN:OE1	1:B:355:LYS:HG3	1.74	0.88
1:A:265:GLU:HG2	1:A:266:PRO:HD2	1.56	0.88
1:A:398:ILE:CD1	1:B:160:PHE:HB3	2.03	0.88
1:B:528:ILE:HG12	1:B:529:PRO:HD2	1.56	0.87
1:A:447:ALA:HB2	1:A:482:LEU:HD21	1.57	0.87
1:A:113:LEU:HD12	1:A:117:TYR:CD1	2.09	0.87
1:A:212:LYS:CD	1:A:218:ASP:OD1	2.23	0.87
1:A:147:GLN:H	1:A:147:GLN:HE21	1.15	0.87
1:B:113:LEU:CD1	1:B:156:TYR:CE1	2.47	0.87
1:B:528:ILE:CG1	1:B:529:PRO:HD2	2.04	0.86
1:A:397:LEU:CD2	1:A:423:VAL:CG1	2.53	0.86
1:A:456:ARG:HH11	1:A:457:ARG:HH22	0.86	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ILE:HG13	4:A:602:HOH:O	1.75	0.86
1:A:405:THR:CG2	1:A:518:GLU:O	2.22	0.86
1:A:86:GLY:O	1:A:117:TYR:CE2	2.29	0.86
1:A:511:ARG:O	1:A:514:ARG:HG2	1.75	0.86
1:B:245:LYS:HZ3	1:B:245:LYS:HB2	1.41	0.86
1:B:397:LEU:CD2	1:B:423:VAL:CG1	2.53	0.85
1:A:447:ALA:O	1:A:451:VAL:HG13	1.76	0.85
1:B:113:LEU:HB3	1:B:156:TYR:CZ	2.11	0.85
1:A:104:GLN:CG	1:A:117:TYR:OH	2.25	0.85
1:A:451:VAL:HG11	1:A:474:ILE:HA	1.59	0.85
1:A:85:ASP:O	1:A:117:TYR:HB2	1.77	0.84
1:A:459:ILE:CD1	1:A:470:ARG:HB2	2.06	0.84
1:B:25:ILE:HD12	4:B:644:HOH:O	1.77	0.84
1:B:113:LEU:HG	1:B:117:TYR:CD1	2.11	0.84
1:A:117:TYR:CD1	1:A:117:TYR:O	2.30	0.84
1:A:196:MET:HE1	1:A:230:HIS:HD2	1.41	0.84
1:B:70:HIS:CE1	1:B:81:ARG:HG2	2.14	0.83
1:A:503:ARG:O	1:A:507:VAL:HG23	1.80	0.82
1:B:98:PRO:O	1:B:99:VAL:CG2	2.27	0.82
1:B:269:PHE:O	1:B:269:PHE:CD2	2.32	0.82
1:A:380:LEU:HD13	1:A:380:LEU:C	2.05	0.82
1:B:302:ILE:O	1:B:305:VAL:HG22	1.80	0.82
1:A:456:ARG:HH11	1:A:457:ARG:NH2	1.60	0.82
1:A:315:GLN:OE1	1:A:355:LYS:HG3	1.79	0.81
1:B:102:PHE:CZ	1:B:137:GLY:HA3	2.14	0.81
1:A:287:ILE:HG12	1:A:287:ILE:O	1.79	0.81
1:A:341:PRO:HG3	1:A:375:ASP:OD2	1.81	0.81
1:B:170:ILE:HG22	1:B:261:ASN:HB3	1.62	0.81
1:B:455:HIS:NE2	1:B:473:LEU:HG	1.95	0.81
1:B:86:GLY:O	1:B:117:TYR:HE2	1.64	0.81
1:A:149:GLY:O	1:B:444:VAL:HG23	1.81	0.81
1:A:113:LEU:O	1:A:145:ARG:HB2	1.79	0.80
1:A:70:HIS:HD2	1:A:72:SER:H	1.30	0.80
1:B:326:PHE:HE1	1:B:363:CYS:SG	2.05	0.80
1:B:398:ILE:HG13	1:B:399:PHE:N	1.95	0.80
1:A:175:LEU:HD22	1:A:177:VAL:HG13	1.63	0.80
1:B:475:GLN:HA	1:B:478:GLU:OE1	1.82	0.80
1:A:520:LEU:HD22	1:B:165:HIS:CD2	2.16	0.79
1:B:200:THR:O	1:B:200:THR:CG2	2.30	0.79
1:A:98:PRO:O	1:A:99:VAL:HG23	1.83	0.79
1:A:149:GLY:O	1:B:444:VAL:CG2	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:MET:CE	1:B:449:GLY:C	2.55	0.79
1:A:371:LEU:HD21	1:A:510:LEU:HD11	1.65	0.79
1:A:113:LEU:HD23	1:A:156:TYR:CZ	2.18	0.79
1:B:23:ARG:O	1:B:23:ARG:CD	2.31	0.78
1:A:113:LEU:HD23	1:A:156:TYR:CE2	2.18	0.78
1:B:113:LEU:CG	1:B:156:TYR:CE1	2.67	0.78
1:B:115:GLU:HG2	1:B:119:GLN:OE1	1.82	0.78
1:A:145:ARG:HD2	1:A:148:GLU:OE2	1.82	0.78
1:A:146:ILE:HG22	1:B:454:LEU:CD1	2.13	0.78
1:A:474:ILE:O	1:A:478:GLU:HG3	1.84	0.78
1:B:35:ARG:O	1:B:39:LYS:HG2	1.85	0.77
1:A:147:GLN:H	1:A:147:GLN:NE2	1.81	0.77
1:B:415:LYS:HG2	1:B:417:PHE:HE2	1.49	0.77
1:A:362:THR:HG23	1:A:366:PHE:HE2	1.50	0.76
1:A:470:ARG:O	1:A:474:ILE:HG13	1.85	0.76
1:A:302:ILE:O	1:A:305:VAL:HG22	1.85	0.76
1:B:445:MET:HE3	1:B:449:GLY:HA3	1.67	0.76
1:B:379:PHE:O	1:B:381:PRO:HD3	1.84	0.76
1:B:23:ARG:HD2	1:B:27:GLU:OE1	1.85	0.76
1:B:121:ILE:O	1:B:125:MET:HG3	1.84	0.76
1:A:160:PHE:HB3	1:B:398:ILE:HD13	1.65	0.76
1:B:316:PRO:HD2	4:B:547:HOH:O	1.85	0.76
1:A:467:GLU:HG3	1:A:470:ARG:NH2	2.01	0.75
1:A:350:ILE:H	1:A:385:GLN:HE22	1.34	0.75
1:A:459:ILE:HD13	1:A:470:ARG:HB2	1.66	0.75
1:A:10:ASP:O	1:A:16:GLY:CA	2.34	0.75
1:A:457:ARG:HH11	1:A:457:ARG:HG2	1.49	0.75
1:A:113:LEU:HD22	1:A:156:TYR:CE1	2.21	0.75
1:A:339:ASN:HB2	1:A:375:ASP:O	1.87	0.75
1:B:409:ILE:HD11	1:B:513:LEU:CD1	2.16	0.75
1:B:10:ASP:CG	1:B:11:ILE:H	1.94	0.74
1:B:113:LEU:HD22	1:B:156:TYR:CD1	2.22	0.74
1:A:520:LEU:CD2	1:B:165:HIS:NE2	2.50	0.74
1:B:80:ASN:C	1:B:82:PRO:HD3	2.13	0.74
1:A:87:VAL:HG12	1:A:117:TYR:CD2	2.21	0.74
1:A:275:LEU:HD21	1:A:507:VAL:HG11	1.68	0.74
1:B:70:HIS:CD2	4:B:566:HOH:O	2.39	0.74
1:A:513:LEU:O	1:A:516:LYS:N	2.20	0.74
1:A:10:ASP:O	1:A:10:ASP:OD1	2.06	0.74
1:A:187:SER:HB3	1:A:188:PRO:CD	2.17	0.74
1:B:70:HIS:CE1	1:B:77:LEU:O	2.41	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PRO:HB2	1:A:343:GLN:HG3	1.68	0.74
1:B:326:PHE:CE1	1:B:363:CYS:SG	2.80	0.74
1:A:227:ALA:HB1	1:A:240:MET:HG3	1.70	0.74
1:A:154:GLY:HA2	1:B:428:HIS:CE1	2.21	0.73
1:B:104:GLN:HG2	1:B:117:TYR:OH	1.88	0.73
1:B:528:ILE:HG12	1:B:529:PRO:CD	2.18	0.73
1:A:316:PRO:HD2	4:A:600:HOH:O	1.89	0.73
1:A:469:THR:O	1:A:472:ARG:HB3	1.89	0.73
1:B:287:ILE:HG23	1:B:288:VAL:N	2.03	0.73
1:A:265:GLU:HG2	1:A:266:PRO:CD	2.19	0.73
1:A:405:THR:O	1:A:516:LYS:CE	2.37	0.72
1:A:146:ILE:CG2	1:B:454:LEU:CD1	2.65	0.72
1:B:158:GLU:OE2	1:B:161:ARG:NH1	2.22	0.72
1:B:339:ASN:CG	1:B:424:MET:HE2	2.14	0.72
1:A:513:LEU:O	1:A:515:THR:N	2.23	0.72
1:B:277:VAL:HG23	1:B:277:VAL:O	1.89	0.72
1:B:23:ARG:O	1:B:23:ARG:HD2	1.89	0.72
1:B:87:VAL:HG12	1:B:117:TYR:CD2	2.25	0.72
1:B:113:LEU:HG	1:B:117:TYR:HD1	1.50	0.72
1:A:193:PHE:HD1	1:A:238:HIS:CD2	2.07	0.71
1:A:398:ILE:HG13	1:A:399:PHE:N	1.98	0.71
1:A:293:ASN:O	1:A:295:PRO:HD3	1.90	0.71
1:A:299:HIS:HE1	1:A:313:GLU:OE2	1.72	0.71
1:B:254:LEU:HD13	1:B:312:PHE:HE2	1.56	0.71
1:A:32:GLY:CA	1:A:107:THR:CG2	2.68	0.71
1:A:113:LEU:CD2	1:A:156:TYR:CE1	2.74	0.70
1:A:215:THR:HG23	1:A:215:THR:O	1.88	0.70
1:B:451:VAL:HB	1:B:455:HIS:HD2	1.55	0.70
1:B:106:PHE:HB2	1:B:140:ASP:OD2	1.91	0.70
1:B:445:MET:HE2	1:B:449:GLY:O	1.91	0.70
1:A:398:ILE:HD13	1:B:160:PHE:HB3	1.71	0.70
1:A:292:ALA:O	1:A:414:ARG:NH1	2.25	0.70
1:A:399:PHE:CD1	1:B:164:THR:HG23	2.27	0.70
1:A:504:ARG:HG2	1:A:508:ARG:HD2	1.72	0.70
1:A:196:MET:O	1:A:240:MET:HA	1.92	0.70
1:B:115:GLU:O	1:B:119:GLN:HG3	1.92	0.70
1:B:298:MET:HG3	1:B:298:MET:O	1.92	0.69
1:B:485:TYR:O	1:B:489:GLU:HG3	1.92	0.69
1:A:344:PHE:O	1:A:345:ALA:HB3	1.91	0.69
1:B:374:VAL:HB	1:B:412:ILE:HA	1.72	0.69
1:A:399:PHE:CE1	1:B:164:THR:HG23	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ASP:HB3	1:B:380:LEU:HD12	1.72	0.69
1:B:193:PHE:HD1	1:B:238:HIS:CD2	2.09	0.69
1:B:102:PHE:CZ	1:B:137:GLY:CA	2.75	0.69
1:B:339:ASN:HD21	1:B:424:MET:CE	2.06	0.69
1:A:329:VAL:O	1:A:330:GLU:HB2	1.92	0.69
1:A:354:GLU:OE2	1:B:392:ARG:NH1	2.21	0.69
1:A:165:HIS:CD2	1:B:520:LEU:HD22	2.28	0.69
1:A:231:ASN:O	1:A:318:PHE:HB2	1.93	0.69
1:B:349:ASP:CB	1:B:380:LEU:CD1	2.68	0.69
1:B:22:ARG:HA	1:B:25:ILE:CG2	2.22	0.69
1:A:36:ALA:HB3	1:A:107:THR:HG23	1.74	0.69
1:A:254:LEU:HD23	1:A:312:PHE:HE2	1.57	0.69
1:B:160:PHE:HE1	1:B:187:SER:HB2	1.57	0.69
1:B:447:ALA:O	1:B:451:VAL:HG13	1.92	0.69
1:A:266:PRO:HG2	1:A:368:VAL:HG22	1.76	0.68
1:A:397:LEU:CD2	1:A:423:VAL:HG12	2.23	0.68
1:A:266:PRO:CG	1:A:368:VAL:HG22	2.24	0.68
1:A:457:ARG:CG	1:A:457:ARG:NH1	2.52	0.68
1:A:524:LYS:HD3	4:B:697:HOH:O	1.93	0.68
1:A:367:ASN:HA	1:A:406:VAL:HG11	1.75	0.68
1:A:32:GLY:CA	1:A:107:THR:HG21	2.22	0.68
1:B:23:ARG:C	1:B:23:ARG:HE	2.01	0.68
1:A:380:LEU:HD13	1:A:380:LEU:O	1.94	0.67
1:B:438:PRO:HD3	1:B:497:ILE:O	1.94	0.67
1:A:113:LEU:CD1	1:A:117:TYR:CD1	2.77	0.67
1:A:407:PRO:HB3	1:A:513:LEU:HD23	1.76	0.67
1:A:455:HIS:O	1:A:459:ILE:HG22	1.95	0.67
1:A:520:LEU:CD2	1:B:165:HIS:CE1	2.77	0.67
1:B:456:ARG:O	1:B:459:ILE:CG2	2.42	0.67
1:A:207:GLY:O	1:A:211:ILE:HG23	1.95	0.67
1:A:485:TYR:O	1:A:489:GLU:HG3	1.94	0.67
1:B:254:LEU:HD13	1:B:312:PHE:CE2	2.29	0.67
1:A:221:PHE:CB	2:A:5600:BTN:H81	2.24	0.67
1:A:120:LYS:O	1:A:124:VAL:HG23	1.94	0.67
1:A:339:ASN:CB	1:A:375:ASP:O	2.43	0.67
1:A:501:ASP:OD1	1:A:501:ASP:O	2.13	0.67
1:B:113:LEU:CB	1:B:156:TYR:OH	2.40	0.67
1:A:181:ALA:CB	1:A:204:PHE:CE1	2.78	0.66
1:B:231:ASN:HD21	1:B:239:HIS:N	1.93	0.66
1:B:241:ALA:CB	1:B:247:ALA:HB2	2.23	0.66
1:B:339:ASN:O	1:B:341:PRO:HD3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ARG:O	1:B:459:ILE:HG23	1.96	0.66
1:A:456:ARG:O	1:A:457:ARG:HG3	1.96	0.66
1:A:482:LEU:N	1:A:482:LEU:HD12	2.10	0.66
1:B:459:ILE:HD13	1:B:470:ARG:HB2	1.77	0.66
1:B:509:GLY:O	1:B:513:LEU:CG	2.41	0.66
1:B:349:ASP:HB3	1:B:380:LEU:CD1	2.26	0.66
1:B:462:ALA:C	1:B:464:ASP:N	2.52	0.66
1:A:117:TYR:CD1	1:A:117:TYR:C	2.74	0.66
1:B:340:GLN:CD	1:B:342:MET:HG3	2.21	0.66
1:B:11:ILE:HG23	1:B:12:HIS:N	2.10	0.66
1:B:407:PRO:HB3	1:B:513:LEU:HB3	1.77	0.66
1:A:406:VAL:HG12	4:B:625:HOH:O	1.95	0.66
1:B:287:ILE:CG2	1:B:288:VAL:N	2.59	0.66
1:A:85:ASP:OD2	1:A:116:VAL:HB	1.96	0.65
1:A:386:GLU:OE2	1:B:204:PHE:HA	1.96	0.65
1:B:392:ARG:CG	1:B:393:ARG:HG3	2.23	0.65
1:A:462:ALA:O	1:A:464:ASP:N	2.29	0.65
1:A:121:ILE:O	1:A:121:ILE:HG22	1.95	0.65
1:A:113:LEU:CD2	1:A:156:TYR:CZ	2.79	0.65
1:B:41:HIS:ND1	4:B:617:HOH:O	2.28	0.65
1:A:119:GLN:O	1:A:119:GLN:NE2	2.30	0.65
1:A:193:PHE:CD1	1:A:238:HIS:CD2	2.84	0.65
1:B:508:ARG:HD3	4:B:637:HOH:O	1.96	0.65
1:A:70:HIS:CE1	1:A:81:ARG:HG2	2.32	0.65
1:A:477:TYR:HD1	1:A:482:LEU:HD11	1.61	0.65
1:B:129:LEU:HD21	1:B:166:ALA:HB2	1.78	0.65
1:A:490:ARG:NH2	1:B:115:GLU:OE1	2.30	0.65
1:B:114:GLY:HA3	1:B:148:GLU:OE2	1.97	0.65
1:B:245:LYS:HB2	1:B:245:LYS:NZ	2.11	0.64
1:A:362:THR:CG2	1:A:366:PHE:CE2	2.81	0.64
1:B:23:ARG:O	1:B:23:ARG:NE	2.30	0.64
1:B:106:PHE:HB2	1:B:140:ASP:CG	2.23	0.64
1:A:362:THR:HG23	1:A:366:PHE:CE2	2.32	0.64
1:B:77:LEU:HD21	1:B:109:PHE:CE1	2.32	0.64
1:B:502:THR:O	1:B:506:ILE:HG12	1.97	0.64
1:B:347:CYS:SG	1:B:377:PRO:CG	2.83	0.64
1:B:113:LEU:HD22	1:B:156:TYR:CZ	2.33	0.64
1:A:392:ARG:HG3	1:A:393:ARG:CG	2.26	0.64
1:B:23:ARG:HH21	1:B:24:ARG:HG3	1.63	0.64
1:B:114:GLY:CA	1:B:148:GLU:OE2	2.45	0.64
1:B:257:TYR:HE1	1:B:328:ARG:NH1	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:HD13	1:B:371:LEU:HB2	1.79	0.64
1:B:402:ALA:HB2	1:B:429:LEU:HD22	1.78	0.64
1:B:528:ILE:HG13	1:B:529:PRO:HD2	1.78	0.63
1:A:520:LEU:HD22	1:B:165:HIS:NE2	2.11	0.63
1:A:126:ASP:OD1	1:A:162:ARG:HD3	1.97	0.63
1:B:457:ARG:HD3	1:B:457:ARG:N	2.14	0.63
1:B:397:LEU:CD2	1:B:423:VAL:HG12	2.29	0.63
1:A:387:HIS:O	1:B:234:SER:CB	2.46	0.63
1:B:26:GLU:O	1:B:30:HIS:HD2	1.81	0.63
1:A:181:ALA:HB2	1:A:204:PHE:CE1	2.33	0.62
1:B:86:GLY:O	1:B:117:TYR:CE2	2.50	0.62
1:A:403:GLU:HA	1:A:520:LEU:HD11	1.81	0.62
1:B:147:GLN:H	1:B:147:GLN:NE2	1.96	0.62
1:B:170:ILE:HG22	1:B:261:ASN:CB	2.30	0.62
1:A:86:GLY:C	1:A:117:TYR:CD2	2.78	0.62
1:A:374:VAL:HB	1:A:412:ILE:HA	1.80	0.62
1:B:455:HIS:O	1:B:457:ARG:N	2.32	0.62
1:B:417:PHE:CE1	1:B:443:ALA:HB3	2.34	0.62
1:A:87:VAL:HG12	1:A:117:TYR:HD2	1.65	0.62
1:A:32:GLY:HA3	1:A:107:THR:HG22	1.80	0.62
1:A:169:VAL:HA	1:A:262:ASN:ND2	2.15	0.62
1:A:459:ILE:HD11	1:A:470:ARG:HB2	1.82	0.62
1:B:455:HIS:CD2	1:B:473:LEU:HG	2.33	0.62
1:A:10:ASP:C	1:A:16:GLY:HA3	2.25	0.62
1:A:125:MET:CE	1:A:163:ASN:ND2	2.63	0.62
1:B:401:TYR:CD2	1:B:423:VAL:O	2.52	0.62
1:A:397:LEU:HD23	1:A:423:VAL:HG12	1.73	0.62
1:A:125:MET:HE1	1:A:163:ASN:ND2	2.15	0.62
1:A:376:VAL:O	1:A:376:VAL:HG13	1.99	0.62
1:B:97:ARG:HB3	1:B:98:PRO:HD2	1.82	0.61
1:B:308:ASP:O	1:B:309:ALA:C	2.43	0.61
1:A:405:THR:O	1:A:516:LYS:NZ	2.32	0.61
1:A:86:GLY:O	1:A:117:TYR:CD2	2.53	0.61
1:A:528:ILE:HG12	1:A:529:PRO:HD2	1.82	0.61
1:B:98:PRO:C	1:B:99:VAL:HG23	2.24	0.61
1:A:117:TYR:O	1:A:117:TYR:CG	2.53	0.61
1:A:147:GLN:HE21	1:A:147:GLN:N	1.94	0.61
1:A:451:VAL:HG21	1:A:474:ILE:CG1	2.26	0.61
1:B:112:ALA:HA	1:B:143:GLY:O	2.01	0.60
1:A:149:GLY:C	1:B:444:VAL:HG23	2.25	0.60
1:A:362:THR:CG2	1:A:366:PHE:HE2	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:CG	1:B:156:TYR:HE1	2.06	0.60
1:B:193:PHE:CD1	1:B:238:HIS:CD2	2.88	0.60
1:A:36:ALA:CB	1:A:107:THR:HG23	2.31	0.60
1:A:475:GLN:CD	1:A:475:GLN:O	2.45	0.60
1:A:392:ARG:CG	1:A:393:ARG:HG3	2.26	0.60
1:A:462:ALA:C	1:A:464:ASP:N	2.58	0.60
1:B:102:PHE:CE1	1:B:137:GLY:HA3	2.36	0.60
1:B:113:LEU:HG	1:B:117:TYR:CE1	2.36	0.60
1:A:32:GLY:CA	1:A:107:THR:HG22	2.31	0.60
1:A:462:ALA:C	1:A:464:ASP:H	2.10	0.60
1:A:525:HIS:ND1	1:A:526:GLY:O	2.35	0.60
1:A:21:LEU:O	1:A:21:LEU:HG	2.01	0.60
1:A:221:PHE:HB2	2:A:5600:BTN:H81	1.84	0.60
1:A:340:GLN:CD	1:A:342:MET:HG3	2.26	0.60
1:B:344:PHE:O	1:B:345:ALA:HB3	2.01	0.60
1:B:462:ALA:C	1:B:464:ASP:H	2.09	0.60
1:A:478:GLU:CB	1:A:482:LEU:HD22	2.32	0.60
1:A:141:SER:O	1:A:179:PRO:HB2	2.00	0.60
1:B:343:GLN:O	1:B:344:PHE:HB2	2.02	0.60
1:B:472:ARG:HH21	1:B:473:LEU:HD11	1.67	0.60
1:B:104:GLN:CG	1:B:117:TYR:OH	2.50	0.59
1:B:339:ASN:ND2	1:B:424:MET:HE2	2.17	0.59
1:A:266:PRO:HB2	1:A:333:PRO:HG2	1.83	0.59
1:A:366:PHE:O	1:A:367:ASN:HB2	2.01	0.59
1:B:269:PHE:O	1:B:269:PHE:HD2	1.82	0.59
1:A:11:ILE:HG23	1:A:12:HIS:N	2.16	0.59
1:A:520:LEU:HD21	1:B:165:HIS:NE2	2.18	0.59
1:B:158:GLU:CD	1:B:161:ARG:HH12	2.11	0.59
1:B:451:VAL:O	1:B:455:HIS:HB2	2.02	0.59
1:A:254:LEU:CD2	1:A:312:PHE:HE2	2.15	0.59
1:A:415:LYS:HE3	1:A:417:PHE:HE2	1.67	0.59
1:A:457:ARG:NH1	1:A:457:ARG:HG3	2.18	0.59
1:B:65:ASP:HB2	1:B:120:LYS:HE3	1.84	0.58
1:B:299:HIS:HE1	1:B:313:GLU:OE2	1.86	0.58
1:B:358:ARG:HG2	4:B:567:HOH:O	2.02	0.58
1:A:169:VAL:HG12	1:A:170:ILE:HG23	1.86	0.58
1:A:215:THR:O	1:A:215:THR:CG2	2.51	0.58
1:B:65:ASP:OD2	1:B:123:LYS:HD2	2.03	0.58
1:B:87:VAL:CG1	1:B:117:TYR:CD2	2.86	0.58
1:A:211:ILE:HD12	1:A:211:ILE:O	2.02	0.58
1:A:386:GLU:HG3	1:A:386:GLU:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:TYR:CD1	1:A:482:LEU:HD11	2.37	0.58
1:B:200:THR:CG2	4:B:631:HOH:O	2.51	0.58
1:A:387:HIS:O	1:A:388:ASP:C	2.45	0.58
1:B:341:PRO:HB3	1:B:414:ARG:NH2	2.19	0.58
1:B:91:TYR:CD1	1:B:91:TYR:C	2.81	0.58
1:A:405:THR:HG22	1:A:518:GLU:O	2.03	0.57
1:A:457:ARG:HH11	1:A:457:ARG:HG3	1.69	0.57
1:A:181:ALA:HB1	1:A:204:PHE:CE1	2.38	0.57
1:B:126:ASP:OD1	1:B:162:ARG:HD3	2.04	0.57
1:B:173:ILE:HD12	1:B:255:LEU:HD21	1.87	0.57
1:B:124:VAL:HG12	1:B:125:MET:N	2.18	0.57
1:B:10:ASP:OD1	1:B:13:THR:HG23	2.05	0.57
1:A:503:ARG:O	1:A:503:ARG:HG2	2.05	0.57
1:B:478:GLU:O	1:B:482:LEU:HB2	2.05	0.57
1:B:113:LEU:HB3	1:B:156:TYR:CE1	2.40	0.57
1:B:214:VAL:HG12	1:B:215:THR:HG22	1.86	0.57
1:A:100:ALA:HB1	1:A:124:VAL:HG12	1.86	0.56
1:B:47:THR:OG1	1:B:50:GLU:HG3	2.04	0.56
1:B:113:LEU:CB	1:B:156:TYR:CE1	2.88	0.56
1:A:303:GLU:O	1:A:309:ALA:HA	2.04	0.56
1:A:315:GLN:HB2	1:A:355:LYS:HE3	1.88	0.56
1:A:477:TYR:O	1:A:482:LEU:CD1	2.53	0.56
1:A:405:THR:O	1:A:516:LYS:HE2	2.04	0.56
1:B:147:GLN:H	1:B:147:GLN:HE21	1.54	0.56
1:B:339:ASN:ND2	1:B:424:MET:CE	2.68	0.56
1:B:314:THR:O	1:B:315:GLN:C	2.49	0.56
1:A:503:ARG:O	1:A:507:VAL:CG2	2.52	0.56
1:A:390:ILE:HG23	1:A:391:ILE:N	2.21	0.56
1:A:433:LEU:HA	1:A:494:ASP:OD1	2.06	0.56
1:B:163:ASN:HB3	1:B:190:ILE:CG2	2.34	0.55
1:A:477:TYR:O	1:A:482:LEU:HD13	2.07	0.55
1:B:271:GLU:O	1:B:271:GLU:HG3	2.07	0.55
1:B:528:ILE:HG12	1:B:529:PRO:N	2.21	0.55
1:B:37:VAL:HG12	1:B:37:VAL:O	2.06	0.55
1:B:193:PHE:CD1	1:B:238:HIS:NE2	2.75	0.55
1:B:308:ASP:O	1:B:310:GLU:N	2.39	0.55
1:A:176:VAL:HB	1:A:196:MET:HG2	1.89	0.55
1:A:211:ILE:HD12	1:A:215:THR:HG22	1.88	0.55
1:A:464:ASP:O	1:A:465:ASP:HB2	2.05	0.55
1:A:390:ILE:HG13	1:B:186:TYR:OH	2.07	0.55
1:B:392:ARG:HG3	1:B:393:ARG:CG	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ILE:O	1:B:147:GLN:C	2.50	0.55
1:B:417:PHE:CD1	1:B:443:ALA:HB3	2.42	0.55
1:A:54:LEU:HD21	1:A:245:LYS:HD2	1.89	0.55
1:A:113:LEU:HD23	1:A:156:TYR:CD2	2.43	0.55
1:B:13:THR:O	1:B:16:GLY:N	2.33	0.55
1:B:102:PHE:CE1	1:B:137:GLY:CA	2.90	0.55
1:B:503:ARG:O	1:B:507:VAL:HG23	2.06	0.55
1:B:24:ARG:O	1:B:67:PHE:HE1	1.90	0.54
1:B:180:CYS:O	1:B:185:VAL:HG12	2.06	0.54
1:A:344:PHE:O	1:A:345:ALA:CB	2.54	0.54
1:A:350:ILE:O	1:A:354:GLU:HG3	2.07	0.54
1:A:70:HIS:HD2	1:A:72:SER:N	2.03	0.54
1:A:87:VAL:CB	1:A:117:TYR:HD2	2.17	0.54
1:B:61:PHE:HE2	1:B:63:GLU:HB2	1.70	0.54
1:B:501:ASP:O	1:B:505:HIS:HD2	1.89	0.54
1:A:379:PHE:HZ	1:A:423:VAL:HG21	1.72	0.54
1:A:409:ILE:CD1	1:A:510:LEU:HG	2.37	0.54
1:B:111:GLY:O	1:B:141:SER:OG	2.23	0.54
1:B:132:GLY:C	1:B:261:ASN:HD22	2.15	0.54
1:B:219:VAL:HG22	1:B:220:GLY:N	2.22	0.54
1:A:458:THR:O	1:A:458:THR:CG2	2.55	0.54
1:B:478:GLU:HA	1:B:482:LEU:HD13	1.88	0.54
1:A:175:LEU:C	1:A:175:LEU:CD2	2.81	0.54
1:A:458:THR:O	1:A:458:THR:HG22	2.08	0.54
1:A:520:LEU:HD22	1:B:165:HIS:CE1	2.42	0.54
1:B:467:GLU:OE1	1:B:467:GLU:N	2.30	0.54
1:A:52:ILE:HD11	1:A:88:VAL:HB	1.89	0.54
1:A:69:ARG:HD2	1:A:83:TYR:CE2	2.43	0.54
1:A:501:ASP:OD1	1:A:504:ARG:HB3	2.08	0.54
1:B:254:LEU:CD1	1:B:312:PHE:HE2	2.21	0.54
1:B:298:MET:O	1:B:302:ILE:HD12	2.08	0.54
1:A:219:VAL:HG22	1:A:223:GLU:HG2	1.90	0.53
1:A:160:PHE:CE1	1:A:187:SER:CB	2.84	0.53
1:A:181:ALA:HB2	1:A:204:PHE:CZ	2.43	0.53
1:B:94:VAL:O	1:B:95:ASP:HB2	2.09	0.53
1:B:158:GLU:HB3	1:B:162:ARG:HH12	1.73	0.53
1:B:403:GLU:HA	1:B:520:LEU:HD11	1.90	0.53
1:B:462:ALA:O	1:B:464:ASP:N	2.41	0.53
1:A:475:GLN:CD	1:A:475:GLN:C	2.77	0.53
1:A:528:ILE:HG12	1:A:529:PRO:CD	2.38	0.53
1:B:253:GLN:O	1:B:256:SER:OG	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD13	1:A:117:TYR:CE1	2.43	0.53
1:A:102:PHE:CZ	1:A:137:GLY:HA3	2.44	0.53
1:A:219:VAL:CG2	1:A:223:GLU:HG2	2.38	0.53
1:A:349:ASP:O	1:A:350:ILE:C	2.52	0.53
1:A:379:PHE:CE1	1:A:420:ALA:HB2	2.43	0.53
1:A:528:ILE:CG1	1:A:529:PRO:HD2	2.38	0.53
1:B:10:ASP:CG	1:B:11:ILE:N	2.64	0.53
1:B:231:ASN:HD21	1:B:238:HIS:C	2.16	0.53
1:A:178:GLY:O	1:A:201:SER:HA	2.09	0.53
1:A:254:LEU:HD23	1:A:312:PHE:CE2	2.42	0.53
1:B:87:VAL:CB	1:B:117:TYR:CE2	2.85	0.53
1:A:478:GLU:HG2	1:A:482:LEU:CD2	2.39	0.53
1:B:277:VAL:O	1:B:277:VAL:CG2	2.57	0.53
1:A:99:VAL:CG2	1:A:134:PRO:HB2	2.32	0.52
1:B:124:VAL:CG1	1:B:125:MET:N	2.71	0.52
1:B:433:LEU:HA	1:B:494:ASP:OD1	2.10	0.52
1:A:230:HIS:CE1	1:B:391:ILE:HD12	2.44	0.52
1:A:447:ALA:CB	1:A:478:GLU:HG2	2.40	0.52
1:B:295:PRO:HB2	1:B:342:MET:HE3	1.90	0.52
1:A:63:GLU:HG2	1:A:66:GLU:HB2	1.91	0.52
1:B:33:SER:O	1:B:36:ALA:N	2.41	0.52
1:A:165:HIS:NE2	1:B:520:LEU:CD2	2.72	0.52
1:A:170:ILE:HG22	1:A:261:ASN:HB3	1.92	0.52
1:A:362:THR:HG22	1:A:366:PHE:CE2	2.45	0.52
1:B:483:ASN:HD22	1:B:483:ASN:C	2.17	0.52
1:B:528:ILE:CG1	1:B:529:PRO:CD	2.79	0.52
1:A:154:GLY:CA	1:B:428:HIS:CE1	2.91	0.52
1:A:188:PRO:O	1:A:191:THR:OG1	2.26	0.52
1:A:456:ARG:CZ	1:A:457:ARG:NH2	2.69	0.52
1:B:445:MET:HE3	1:B:449:GLY:CA	2.40	0.52
1:A:94:VAL:O	1:A:95:ASP:HB2	2.10	0.52
1:B:69:ARG:NH1	1:B:83:TYR:OH	2.43	0.52
1:B:180:CYS:O	1:B:185:VAL:CG1	2.57	0.52
1:A:234:SER:HA	1:B:387:HIS:O	2.10	0.52
1:A:482:LEU:CD1	1:A:482:LEU:N	2.73	0.52
1:A:483:ASN:C	1:A:483:ASN:HD22	2.17	0.52
1:A:275:LEU:CD2	1:A:507:VAL:HG21	2.40	0.51
1:A:438:PRO:HD3	1:A:497:ILE:O	2.10	0.51
1:B:11:ILE:CG2	1:B:12:HIS:N	2.72	0.51
1:B:23:ARG:C	1:B:23:ARG:NE	2.68	0.51
1:A:145:ARG:CD	1:A:148:GLU:OE2	2.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:O	1:B:141:SER:CB	2.59	0.51
1:B:324:THR:HA	1:B:336:ILE:O	2.10	0.51
1:A:113:LEU:CD1	1:A:117:TYR:HD1	2.10	0.51
1:A:340:GLN:OE1	1:A:342:MET:HG3	2.11	0.51
1:A:381:PRO:HG2	1:B:214:VAL:HG11	1.92	0.51
1:B:326:PHE:CZ	1:B:359:PHE:CE1	2.98	0.51
1:A:70:HIS:HA	1:A:116:VAL:HG21	1.92	0.51
1:B:457:ARG:CG	1:B:457:ARG:NH1	2.38	0.51
1:A:134:PRO:HG3	1:A:171:PRO:HG2	1.91	0.51
1:B:160:PHE:CE1	1:B:187:SER:HB2	2.44	0.51
1:A:380:LEU:O	1:A:380:LEU:CD1	2.59	0.51
1:B:70:HIS:CD2	1:B:70:HIS:C	2.88	0.51
1:A:380:LEU:C	1:A:380:LEU:CD1	2.77	0.50
1:A:451:VAL:HG11	1:A:474:ILE:CA	2.37	0.50
1:A:455:HIS:O	1:A:459:ILE:CG2	2.58	0.50
1:B:401:TYR:CE2	1:B:423:VAL:O	2.64	0.50
1:A:498:MET:O	1:A:499:PRO:C	2.54	0.50
1:B:40:GLN:HE22	1:B:45:LYS:NZ	2.10	0.50
1:A:299:HIS:O	1:A:303:GLU:HG3	2.11	0.50
1:A:444:VAL:HA	1:B:153:LEU:HD11	1.93	0.50
1:B:367:ASN:HA	1:B:406:VAL:HG11	1.92	0.50
1:A:211:ILE:HD12	1:A:215:THR:CG2	2.42	0.50
1:A:380:LEU:HD11	4:A:623:HOH:O	2.10	0.50
1:A:69:ARG:NH1	1:A:83:TYR:CZ	2.79	0.50
1:A:234:SER:HB2	1:A:236:VAL:HG23	1.94	0.50
1:B:91:TYR:CD1	1:B:91:TYR:O	2.65	0.50
1:B:467:GLU:H	1:B:467:GLU:CD	2.17	0.50
1:A:176:VAL:HB	1:A:196:MET:CG	2.41	0.50
1:A:467:GLU:N	1:A:467:GLU:OE2	2.45	0.50
1:B:208:PRO:HD2	1:B:221:PHE:CZ	2.47	0.50
1:A:160:PHE:HE1	1:A:187:SER:CB	2.08	0.50
1:A:478:GLU:HA	1:A:482:LEU:CG	2.40	0.50
1:B:305:VAL:HG23	1:B:306:LEU:N	2.26	0.50
1:A:91:TYR:CD1	1:A:91:TYR:C	2.89	0.49
1:A:232:SER:O	1:A:318:PHE:HD1	1.95	0.49
1:A:475:GLN:O	1:A:475:GLN:OE1	2.30	0.49
1:A:406:VAL:O	1:A:408:LEU:HG	2.13	0.49
1:B:13:THR:O	1:B:14:THR:C	2.55	0.49
1:B:25:ILE:O	1:B:25:ILE:HG13	2.09	0.49
1:A:207:GLY:O	1:A:211:ILE:CG2	2.60	0.49
1:A:60:SER:O	1:A:61:PHE:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:HB3	1:A:162:ARG:HH12	1.76	0.49
1:A:250:TYR:CE1	1:A:312:PHE:CZ	3.00	0.49
1:A:434:ASN:HB3	4:A:656:HOH:O	2.12	0.49
1:B:300:SER:O	1:B:304:HIS:ND1	2.40	0.49
1:B:349:ASP:O	1:B:350:ILE:C	2.55	0.49
1:B:456:ARG:C	1:B:459:ILE:HG22	2.37	0.49
1:A:80:ASN:N	1:A:80:ASN:ND2	2.61	0.49
1:A:121:ILE:O	1:A:125:MET:HG3	2.12	0.49
1:A:198:ASP:CG	1:A:199:GLN:HG2	2.36	0.49
1:A:387:HIS:O	1:B:234:SER:HB2	2.12	0.49
1:A:483:ASN:CB	1:A:484:PRO:HD2	2.31	0.49
1:B:232:SER:O	1:B:318:PHE:HD1	1.95	0.49
1:B:435:LEU:HD13	1:B:435:LEU:N	2.27	0.49
1:B:445:MET:CE	1:B:449:GLY:CA	2.90	0.49
1:B:465:ASP:O	1:B:469:THR:HG23	2.12	0.49
1:A:113:LEU:CD1	1:A:117:TYR:CE1	2.95	0.49
1:A:324:THR:HA	1:A:336:ILE:O	2.13	0.49
1:B:198:ASP:CG	1:B:199:GLN:HG2	2.35	0.49
1:B:226:GLY:O	1:B:229:THR:HB	2.13	0.49
1:B:329:VAL:O	1:B:330:GLU:HB2	2.12	0.49
1:A:265:GLU:CG	1:A:266:PRO:CD	2.90	0.49
1:B:36:ALA:HA	1:B:39:LYS:HG3	1.94	0.49
1:B:147:GLN:HE21	1:B:147:GLN:N	2.11	0.49
1:A:183:GLY:O	1:A:184:ALA:C	2.54	0.49
1:B:445:MET:CE	1:B:449:GLY:HA3	2.41	0.49
1:A:11:ILE:CG2	1:A:12:HIS:N	2.75	0.49
1:A:121:ILE:O	1:A:121:ILE:CG2	2.61	0.48
1:A:230:HIS:HE1	1:B:391:ILE:HD12	1.77	0.48
1:A:517:ARG:HD2	4:A:664:HOH:O	2.12	0.48
1:B:390:ILE:HG23	1:B:391:ILE:N	2.28	0.48
1:A:340:GLN:HG3	1:A:340:GLN:O	2.12	0.48
1:B:113:LEU:HA	1:B:117:TYR:CD1	2.48	0.48
1:B:466:ALA:O	1:B:467:GLU:C	2.56	0.48
1:B:473:LEU:HA	1:B:476:GLU:HG3	1.95	0.48
1:A:435:LEU:N	1:A:435:LEU:HD13	2.27	0.48
1:B:268:ALA:CB	1:B:332:ARG:HG3	2.43	0.48
1:B:364:ASP:CG	1:B:404:ALA:HA	2.38	0.48
1:B:437:TRP:NE1	1:B:502:THR:OG1	2.46	0.48
1:A:391:ILE:HA	1:B:186:TYR:CE1	2.48	0.48
1:B:113:LEU:HD13	1:B:156:TYR:CD1	2.41	0.48
1:B:208:PRO:CD	1:B:221:PHE:CE1	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLU:O	1:B:283:GLU:HB2	2.13	0.48
1:B:434:ASN:C	1:B:435:LEU:HD13	2.38	0.48
1:A:395:ALA:C	1:A:398:ILE:HG23	2.33	0.48
1:B:455:HIS:O	1:B:456:ARG:C	2.56	0.48
1:A:158:GLU:CD	1:A:161:ARG:HH12	2.21	0.48
1:A:170:ILE:HG22	1:A:261:ASN:CB	2.43	0.48
1:A:392:ARG:HG3	1:A:393:ARG:N	2.28	0.48
1:A:409:ILE:HD11	1:A:510:LEU:HG	1.95	0.48
1:B:37:VAL:O	1:B:37:VAL:CG1	2.61	0.48
1:A:193:PHE:HA	1:A:238:HIS:ND1	2.28	0.48
1:A:196:MET:HE1	1:A:230:HIS:CD2	2.34	0.48
1:A:288:VAL:HG11	1:A:439:THR:HG21	1.95	0.48
1:A:459:ILE:HD11	1:A:466:ALA:O	2.14	0.48
1:B:61:PHE:CE2	1:B:63:GLU:HB2	2.48	0.48
1:A:11:ILE:C	1:A:13:THR:H	2.21	0.47
1:B:455:HIS:CE1	1:B:473:LEU:HG	2.50	0.47
1:A:85:ASP:O	1:A:117:TYR:CB	2.57	0.47
1:A:147:GLN:HG3	1:B:454:LEU:CD2	2.43	0.47
1:A:159:ILE:HG22	1:A:163:ASN:OD1	2.14	0.47
1:A:513:LEU:C	1:A:515:THR:N	2.71	0.47
1:B:23:ARG:NH2	1:B:24:ARG:HG3	2.29	0.47
1:B:187:SER:HB3	1:B:188:PRO:CD	2.35	0.47
1:B:188:PRO:O	1:B:191:THR:OG1	2.31	0.47
1:B:266:PRO:CG	1:B:368:VAL:HG22	2.44	0.47
1:B:320:PRO:HB2	1:B:343:GLN:HG3	1.96	0.47
1:A:10:ASP:O	1:A:10:ASP:CG	2.57	0.47
1:A:134:PRO:HG3	1:A:171:PRO:CG	2.45	0.47
1:A:493:VAL:O	1:A:494:ASP:C	2.58	0.47
1:A:56:LEU:HD11	1:A:101:VAL:HG11	1.96	0.47
1:A:445:MET:HE3	1:B:146:ILE:HD12	1.97	0.47
1:B:132:GLY:HA3	1:B:261:ASN:ND2	2.29	0.47
1:B:173:ILE:HD12	1:B:255:LEU:CD2	2.43	0.47
1:A:86:GLY:C	1:A:117:TYR:HD2	2.22	0.47
1:A:113:LEU:HD13	1:A:117:TYR:HE1	1.78	0.47
1:A:170:ILE:HG13	1:A:170:ILE:O	2.15	0.47
1:A:306:LEU:HD21	1:A:336:ILE:HD11	1.96	0.47
1:A:339:ASN:OD1	1:A:424:MET:HE2	2.14	0.47
1:A:389:GLY:O	1:A:393:ARG:HG3	2.13	0.47
1:A:451:VAL:HG23	1:A:452:ASN:N	2.29	0.47
1:A:478:GLU:HG2	1:A:482:LEU:HD22	1.97	0.47
1:B:318:PHE:O	1:B:355:LYS:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ARG:HE	1:B:473:LEU:HD13	1.79	0.47
1:B:287:ILE:HG12	1:B:296:TYR:CD2	2.50	0.47
1:B:474:ILE:O	1:B:478:GLU:OE1	2.32	0.47
1:A:48:ALA:O	1:A:52:ILE:HG13	2.14	0.47
1:B:322:ILE:CG2	1:B:355:LYS:HD3	2.45	0.47
1:B:457:ARG:C	1:B:459:ILE:N	2.71	0.47
1:A:13:THR:O	1:A:16:GLY:N	2.48	0.46
1:A:193:PHE:CE2	1:A:362:THR:HG21	2.50	0.46
1:B:170:ILE:O	1:B:170:ILE:HG13	2.15	0.46
1:A:10:ASP:N	1:A:13:THR:HG23	2.29	0.46
1:A:186:TYR:OH	1:B:390:ILE:HG13	2.14	0.46
1:A:227:ALA:HB3	4:A:571:HOH:O	2.14	0.46
1:A:350:ILE:HG13	1:A:385:GLN:NE2	2.30	0.46
1:A:390:ILE:CG1	1:B:186:TYR:OH	2.63	0.46
1:B:25:ILE:CD1	4:B:644:HOH:O	2.45	0.46
1:B:98:PRO:C	1:B:99:VAL:CG2	2.87	0.46
1:B:401:TYR:CE2	1:B:425:GLY:N	2.83	0.46
1:A:503:ARG:O	1:A:503:ARG:CG	2.63	0.46
1:B:204:PHE:CE1	1:B:207:GLY:HA2	2.51	0.46
1:B:221:PHE:CB	2:B:5601:BTN:H81	2.45	0.46
1:B:284:LEU:HD21	1:B:304:HIS:CG	2.51	0.46
1:A:284:LEU:HG	1:A:304:HIS:CD2	2.50	0.46
1:A:386:GLU:OE2	1:B:204:PHE:CA	2.63	0.46
1:A:389:GLY:O	1:A:393:ARG:CG	2.64	0.46
1:B:221:PHE:HB2	2:B:5601:BTN:H81	1.97	0.46
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.75	0.46
1:B:395:ALA:O	1:B:398:ILE:HG23	2.15	0.46
1:B:445:MET:CE	1:B:449:GLY:O	2.57	0.46
1:A:87:VAL:N	1:A:117:TYR:HD2	2.13	0.46
1:A:302:ILE:O	1:A:305:VAL:CG2	2.61	0.46
1:A:513:LEU:C	1:A:515:THR:H	2.23	0.46
1:B:376:VAL:O	1:B:376:VAL:HG13	2.15	0.46
1:A:102:PHE:CE1	1:A:137:GLY:HA3	2.51	0.46
1:B:193:PHE:HA	1:B:238:HIS:ND1	2.26	0.46
1:B:457:ARG:O	1:B:460:ALA:N	2.48	0.46
1:A:128:ALA:HB1	1:A:133:CYS:O	2.16	0.46
1:A:469:THR:O	1:A:472:ARG:CB	2.61	0.46
1:A:522:PRO:O	1:A:523:LYS:HB3	2.16	0.46
1:A:398:ILE:HD11	1:B:160:PHE:HB3	1.93	0.46
1:A:520:LEU:HD22	1:B:165:HIS:CG	2.50	0.46
1:B:128:ALA:CB	1:B:135:VAL:CG2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ARG:C	1:B:459:ILE:H	2.22	0.46
1:A:454:LEU:HD13	1:B:75:PHE:CZ	2.51	0.46
1:B:116:VAL:O	1:B:120:LYS:N	2.46	0.46
1:A:361:ARG:NH2	4:A:532:HOH:O	2.38	0.45
1:A:498:MET:O	1:A:500:SER:N	2.49	0.45
1:B:187:SER:H	1:B:188:PRO:HD2	1.81	0.45
1:B:198:ASP:OD1	1:B:199:GLN:N	2.49	0.45
1:B:456:ARG:O	1:B:459:ILE:HG22	2.14	0.45
1:A:284:LEU:HD21	1:A:304:HIS:CG	2.51	0.45
1:A:528:ILE:HG12	1:A:529:PRO:N	2.31	0.45
1:B:266:PRO:HG3	1:B:368:VAL:HG22	1.99	0.45
1:A:125:MET:HE3	1:A:163:ASN:ND2	2.32	0.45
1:B:69:ARG:NH1	1:B:83:TYR:CZ	2.84	0.45
1:B:341:PRO:HB3	1:B:414:ARG:HH22	1.81	0.45
1:B:468:ALA:C	1:B:470:ARG:H	2.24	0.45
1:A:146:ILE:CB	1:B:454:LEU:HD11	2.44	0.45
1:A:165:HIS:CD2	1:B:520:LEU:CD2	2.96	0.45
1:A:256:SER:O	1:A:267:PRO:HG2	2.17	0.45
1:A:477:TYR:C	1:A:482:LEU:HD13	2.41	0.45
1:A:493:VAL:O	1:A:493:VAL:HG23	2.17	0.45
1:B:231:ASN:ND2	1:B:238:HIS:C	2.74	0.45
1:A:26:GLU:O	1:A:30:HIS:HD2	1.99	0.45
1:A:113:LEU:CD2	1:A:156:TYR:CD1	2.99	0.45
1:A:322:ILE:HG13	1:A:338:ALA:O	2.16	0.45
1:A:512:GLN:O	1:A:513:LEU:C	2.58	0.45
1:B:87:VAL:HB	1:B:117:TYR:HE2	1.74	0.45
1:B:401:TYR:CZ	1:B:425:GLY:N	2.85	0.45
1:A:102:PHE:CZ	1:A:137:GLY:CA	2.99	0.45
1:A:486:THR:HB	4:A:565:HOH:O	2.16	0.45
1:B:195:VAL:CG2	1:B:247:ALA:HB1	2.47	0.45
1:B:456:ARG:HE	1:B:456:ARG:HB2	1.42	0.45
1:A:483:ASN:C	1:A:483:ASN:ND2	2.75	0.45
1:B:56:LEU:CD1	1:B:61:PHE:HD1	2.30	0.45
1:A:99:VAL:HG22	1:A:134:PRO:CB	2.32	0.45
1:A:175:LEU:HD22	1:A:175:LEU:C	2.42	0.45
1:B:72:SER:O	1:B:78:ASP:HB3	2.16	0.45
1:B:158:GLU:O	1:B:162:ARG:NH1	2.47	0.45
1:B:474:ILE:O	1:B:478:GLU:HG3	2.17	0.45
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.99	0.45
1:A:327:GLY:O	1:A:328:ARG:HG2	2.17	0.45
1:A:436:ALA:O	1:A:496:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ALA:HB2	1:B:135:VAL:CG2	2.46	0.45
1:B:483:ASN:C	1:B:483:ASN:ND2	2.74	0.45
1:B:483:ASN:HB2	1:B:484:PRO:HD2	1.98	0.45
1:A:262:ASN:OD1	1:A:262:ASN:O	2.36	0.44
1:A:389:GLY:O	1:A:393:ARG:HD3	2.16	0.44
1:B:321:ASN:OD1	1:B:321:ASN:N	2.47	0.44
1:B:399:PHE:O	1:B:399:PHE:CD2	2.69	0.44
1:A:156:TYR:HB3	1:A:160:PHE:CE2	2.52	0.44
1:B:399:PHE:CD2	1:B:399:PHE:C	2.95	0.44
1:A:161:ARG:NH2	1:A:162:ARG:NH2	2.65	0.44
1:A:395:ALA:O	1:A:396:LYS:C	2.59	0.44
1:A:478:GLU:HB3	1:A:482:LEU:HD22	1.98	0.44
1:B:40:GLN:HE22	1:B:45:LYS:HZ1	1.63	0.44
1:B:363:CYS:HB3	1:B:368:VAL:HB	1.98	0.44
1:A:86:GLY:O	1:A:117:TYR:HE2	1.96	0.44
1:A:113:LEU:O	1:A:145:ARG:CB	2.57	0.44
1:A:329:VAL:O	1:A:330:GLU:CB	2.64	0.44
1:B:187:SER:N	1:B:188:PRO:CD	2.80	0.44
1:A:262:ASN:OD1	1:A:262:ASN:C	2.58	0.44
1:A:288:VAL:HG22	1:A:296:TYR:CZ	2.53	0.44
1:A:314:THR:O	1:A:315:GLN:C	2.60	0.44
1:B:70:HIS:HD2	1:B:72:SER:N	2.16	0.44
1:B:427:LYS:HB2	1:B:427:LYS:HE2	1.73	0.44
1:A:215:THR:CG2	1:A:217:GLU:HB3	2.47	0.44
1:A:376:VAL:O	1:A:376:VAL:CG1	2.64	0.44
1:A:433:LEU:HD12	1:A:494:ASP:OD1	2.18	0.44
1:A:483:ASN:HB2	1:A:484:PRO:CD	2.35	0.44
1:A:520:LEU:O	1:A:521:PRO:C	2.60	0.44
1:B:198:ASP:HA	1:B:227:ALA:HB3	2.00	0.44
1:B:493:VAL:HG23	1:B:493:VAL:O	2.16	0.44
1:A:182:GLY:O	1:A:185:VAL:HG22	2.18	0.44
1:A:448:GLN:O	1:A:452:ASN:OD1	2.36	0.44
1:B:469:THR:O	1:B:473:LEU:HD22	2.18	0.44
1:B:473:LEU:HA	1:B:473:LEU:HD12	1.80	0.44
1:A:21:LEU:O	1:A:21:LEU:CG	2.65	0.43
1:A:102:PHE:CE1	1:A:137:GLY:CA	3.01	0.43
1:A:231:ASN:HD21	1:A:239:HIS:C	2.26	0.43
1:A:456:ARG:HD2	1:A:457:ARG:CZ	2.48	0.43
1:A:478:GLU:CG	1:A:482:LEU:HD22	2.47	0.43
1:B:130:LYS:HE3	1:B:130:LYS:HB2	1.67	0.43
1:B:204:PHE:CZ	1:B:221:PHE:HE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PRO:HD2	1:B:221:PHE:CE1	2.52	0.43
1:B:212:LYS:O	1:B:213:THR:C	2.61	0.43
1:A:212:LYS:CE	1:A:218:ASP:OD1	2.67	0.43
1:B:182:GLY:O	1:B:185:VAL:HG22	2.18	0.43
1:B:183:GLY:O	1:B:184:ALA:C	2.60	0.43
1:B:326:PHE:CE2	1:B:359:PHE:HE1	2.35	0.43
1:A:475:GLN:O	1:A:475:GLN:CG	2.66	0.43
1:B:344:PHE:O	1:B:345:ALA:CB	2.66	0.43
1:B:284:LEU:HG	1:B:304:HIS:CD2	2.53	0.43
1:B:466:ALA:C	1:B:468:ALA:N	2.70	0.43
1:B:205:ILE:H	1:B:205:ILE:HG13	1.30	0.43
1:B:478:GLU:HG2	1:B:482:LEU:HD22	1.99	0.43
1:A:433:LEU:HA	1:A:433:LEU:HD12	1.80	0.43
1:A:478:GLU:HA	1:A:482:LEU:CD2	2.49	0.43
1:B:78:ASP:O	1:B:78:ASP:CG	2.62	0.43
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.83	0.43
1:A:445:MET:SD	1:A:449:GLY:O	2.77	0.43
1:B:77:LEU:HD21	1:B:109:PHE:CZ	2.54	0.43
1:B:219:VAL:HG22	1:B:220:GLY:O	2.18	0.43
1:B:280:GLU:O	1:B:281:ASP:C	2.61	0.43
1:A:160:PHE:HB3	1:B:398:ILE:CD1	2.43	0.43
1:A:212:LYS:O	1:A:216:GLY:N	2.46	0.43
1:A:250:TYR:CZ	1:A:312:PHE:CZ	3.07	0.43
1:A:386:GLU:CD	1:B:204:PHE:HA	2.43	0.43
1:A:443:ALA:O	1:A:444:VAL:C	2.62	0.43
1:B:200:THR:HG21	4:B:631:HOH:O	2.17	0.43
1:A:478:GLU:HA	1:A:482:LEU:HD22	1.99	0.43
1:B:364:ASP:OD1	1:B:405:THR:N	2.48	0.43
1:B:419:GLY:O	1:B:423:VAL:HG23	2.19	0.43
1:A:337:VAL:O	1:A:372:THR:HA	2.18	0.43
1:A:343:GLN:O	1:A:344:PHE:HB2	2.19	0.43
1:A:409:ILE:HD12	1:A:510:LEU:HG	2.00	0.43
1:A:504:ARG:CG	1:A:508:ARG:HD2	2.45	0.43
1:B:40:GLN:NE2	1:B:45:LYS:NZ	2.66	0.43
1:B:234:SER:C	1:B:236:VAL:H	2.27	0.43
1:B:266:PRO:CD	1:B:367:ASN:O	2.67	0.43
1:B:468:ALA:C	1:B:470:ARG:N	2.75	0.43
1:B:472:ARG:O	1:B:476:GLU:HG3	2.19	0.43
1:A:187:SER:CB	1:A:188:PRO:HD3	2.21	0.42
1:B:81:ARG:N	1:B:82:PRO:HD3	2.29	0.42
1:A:148:GLU:O	1:A:151:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CD2	1:A:177:VAL:HG13	2.42	0.42
1:B:85:ASP:O	1:B:117:TYR:HD2	2.02	0.42
1:A:520:LEU:CD2	1:B:165:HIS:CD2	2.94	0.42
1:B:20:ASP:HB3	4:B:539:HOH:O	2.19	0.42
1:B:125:MET:HE1	1:B:163:ASN:ND2	2.33	0.42
1:B:315:GLN:HB2	1:B:355:LYS:HE3	2.01	0.42
1:B:332:ARG:NH2	1:B:514:ARG:HH12	2.17	0.42
1:A:387:HIS:O	1:B:234:SER:HA	2.19	0.42
1:A:390:ILE:O	1:A:391:ILE:C	2.62	0.42
1:B:198:ASP:O	1:B:199:GLN:HB2	2.19	0.42
1:A:466:ALA:O	1:A:469:THR:OG1	2.33	0.42
1:B:169:VAL:HG12	1:B:170:ILE:HG23	2.02	0.42
1:B:399:PHE:CG	1:B:528:ILE:HG13	2.54	0.42
1:A:127:PHE:CD2	1:A:127:PHE:C	2.98	0.42
1:A:192:ASP:O	1:A:238:HIS:CE1	2.72	0.42
1:A:383:VAL:O	1:A:384:ASP:C	2.62	0.42
1:B:146:ILE:HG23	1:B:147:GLN:N	2.34	0.42
1:B:228:ARG:O	1:B:229:THR:C	2.62	0.42
1:B:390:ILE:O	1:B:394:GLY:N	2.43	0.42
1:A:146:ILE:HG21	1:B:454:LEU:CD1	2.45	0.42
1:A:152:SER:O	1:A:156:TYR:CD2	2.72	0.42
1:A:87:VAL:HG21	1:A:121:ILE:HD11	2.01	0.42
1:A:215:THR:C	1:A:217:GLU:N	2.78	0.42
1:A:226:GLY:O	1:A:227:ALA:C	2.63	0.42
1:A:459:ILE:HG13	1:A:459:ILE:O	2.20	0.42
1:A:483:ASN:HD22	1:A:483:ASN:N	2.18	0.42
1:B:234:SER:O	1:B:236:VAL:N	2.53	0.42
1:B:341:PRO:HG3	1:B:375:ASP:OD2	2.19	0.42
1:B:364:ASP:OD1	1:B:404:ALA:HA	2.19	0.42
1:B:521:PRO:HA	1:B:522:PRO:HD3	1.93	0.42
1:A:161:ARG:HB2	1:B:429:LEU:HD23	2.01	0.42
1:A:215:THR:C	1:A:217:GLU:H	2.26	0.42
1:A:451:VAL:CG2	1:A:474:ILE:HG12	2.37	0.42
1:B:113:LEU:CG	1:B:117:TYR:CE1	3.02	0.42
1:A:279:ASP:O	1:A:283:GLU:HG3	2.20	0.41
1:B:22:ARG:HA	1:B:25:ILE:HG23	1.99	0.41
1:B:363:CYS:O	1:B:368:VAL:O	2.38	0.41
1:A:113:LEU:HD23	1:A:156:TYR:CE1	2.43	0.41
1:A:340:GLN:O	1:A:341:PRO:C	2.63	0.41
1:B:128:ALA:HB1	1:B:170:ILE:HD12	2.03	0.41
1:A:40:GLN:HE22	1:A:45:LYS:NZ	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:HIS:O	1:A:389:GLY:N	2.54	0.41
1:B:64:LEU:O	1:B:65:ASP:C	2.64	0.41
1:B:523:LYS:HE2	1:B:523:LYS:HB3	1.87	0.41
1:A:266:PRO:O	1:A:267:PRO:C	2.62	0.41
1:B:265:GLU:O	1:B:266:PRO:C	2.63	0.41
1:B:435:LEU:N	1:B:435:LEU:CD1	2.83	0.41
1:A:358:ARG:CG	1:A:358:ARG:O	2.68	0.41
1:A:403:GLU:HA	1:A:520:LEU:CD1	2.49	0.41
1:B:133:CYS:HA	1:B:134:PRO:HD3	1.74	0.41
1:B:302:ILE:O	1:B:305:VAL:CG2	2.60	0.41
1:B:462:ALA:O	1:B:463:GLY:C	2.64	0.41
1:A:406:VAL:O	1:A:407:PRO:C	2.63	0.41
1:A:478:GLU:HG2	1:A:482:LEU:HD21	2.02	0.41
1:B:318:PHE:O	1:B:319:ALA:HB3	2.20	0.41
1:A:69:ARG:NH1	1:A:83:TYR:OH	2.54	0.41
1:A:134:PRO:CB	1:A:171:PRO:HG2	2.51	0.41
1:A:154:GLY:HA2	1:B:428:HIS:NE2	2.36	0.41
1:A:211:ILE:O	1:A:215:THR:HG22	2.20	0.41
1:A:248:VAL:HG12	1:A:252:LYS:HD2	2.02	0.41
1:A:256:SER:HA	4:A:666:HOH:O	2.19	0.41
1:A:325:GLY:O	1:A:359:PHE:HZ	2.04	0.41
1:A:380:LEU:HD13	1:A:381:PRO:O	2.21	0.41
1:B:47:THR:O	1:B:51:ARG:HD2	2.20	0.41
1:B:59:GLY:O	1:B:60:SER:C	2.64	0.41
1:B:100:ALA:O	1:B:135:VAL:HA	2.21	0.41
1:B:192:ASP:O	1:B:238:HIS:CE1	2.74	0.41
1:B:195:VAL:HG11	1:B:251:VAL:HG22	2.03	0.41
1:A:366:PHE:O	1:A:367:ASN:CB	2.65	0.41
1:A:414:ARG:O	1:A:441:GLN:N	2.43	0.41
1:B:102:PHE:CE1	1:B:137:GLY:HA2	2.55	0.41
1:B:417:PHE:CZ	1:B:441:GLN:HB2	2.56	0.41
1:B:451:VAL:HB	1:B:455:HIS:CD2	2.45	0.41
1:A:406:VAL:HB	1:A:407:PRO:HD2	2.03	0.40
1:A:11:ILE:O	1:A:17:LYS:HG3	2.21	0.40
1:A:203:MET:O	1:A:225:GLY:HA3	2.21	0.40
1:A:284:LEU:CD2	1:A:304:HIS:CD2	3.05	0.40
1:A:451:VAL:O	1:A:452:ASN:C	2.64	0.40
1:B:114:GLY:HA2	1:B:148:GLU:CD	2.46	0.40
1:B:166:ALA:O	1:B:169:VAL:N	2.47	0.40
1:B:308:ASP:C	1:B:310:GLU:N	2.74	0.40
1:A:377:PRO:HA	1:A:417:PHE:HD2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:C	1:A:482:LEU:HD12	2.45	0.40
1:B:266:PRO:HD3	1:B:367:ASN:O	2.21	0.40
1:B:287:ILE:CG2	1:B:288:VAL:H	2.32	0.40
1:B:340:GLN:O	1:B:340:GLN:HG3	2.20	0.40
1:B:430:GLY:O	4:B:581:HOH:O	2.21	0.40
1:B:504:ARG:HH11	1:B:508:ARG:HH11	1.69	0.40
1:B:98:PRO:O	1:B:99:VAL:HG22	2.19	0.40
1:A:70:HIS:CE1	1:A:77:LEU:O	2.74	0.40
1:A:287:ILE:O	1:A:287:ILE:CG1	2.58	0.40
1:A:364:ASP:CG	1:A:404:ALA:HA	2.47	0.40
1:B:20:ASP:OD1	1:B:23:ARG:NH2	2.54	0.40
1:B:483:ASN:HD22	1:B:483:ASN:N	2.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/530 (98%)	459 (88%)	58 (11%)	2 (0%)	30	27
1	B	519/530 (98%)	458 (88%)	60 (12%)	1 (0%)	43	42
All	All	1038/1060 (98%)	917 (88%)	118 (11%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	GLY
1	A	514	ARG
1	B	98	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	412/421 (98%)	364 (88%)	48 (12%)	5	3
1	B	412/421 (98%)	373 (90%)	39 (10%)	8	5
All	All	824/842 (98%)	737 (89%)	87 (11%)	6	4

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	35	ARG
1	A	40	GLN
1	A	43	LYS
1	A	47	THR
1	A	53	ASP
1	A	54	LEU
1	A	80	ASN
1	A	99	VAL
1	A	117	TYR
1	A	119	GLN
1	A	124	VAL
1	A	129	LEU
1	A	147	GLN
1	A	175	LEU
1	A	205	ILE
1	A	209	ASP
1	A	211	ILE
1	A	213	THR
1	A	215	THR
1	A	219	VAL
1	A	223	GLU
1	A	232	SER
1	A	245	LYS
1	A	263	LEU
1	A	264	SER
1	A	271	GLU

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Mol	Chain	Res	Type
1	A	275	LEU
1	A	287	ILE
1	A	291	SER
1	A	336	ILE
1	A	342	MET
1	A	380	LEU
1	A	398	ILE
1	A	415	LYS
1	A	433	LEU
1	A	435	LEU
1	A	444	VAL
1	A	453	ILE
1	A	457	ARG
1	A	458	THR
1	A	482	LEU
1	A	483	ASN
1	A	500	SER
1	A	508	ARG
1	A	513	LEU
1	A	517	ARG
1	A	528	ILE
1	B	23	ARG
1	B	25	ILE
1	B	35	ARG
1	B	39	LYS
1	B	40	GLN
1	B	45	LYS
1	B	49	ARG
1	B	54	LEU
1	B	71	ARG
1	B	77	LEU
1	B	124	VAL
1	B	146	ILE
1	B	147	GLN
1	B	177	VAL
1	B	195	VAL
1	B	200	THR
1	B	205	ILE
1	B	212	LYS
1	B	213	THR
1	B	232	SER
1	B	245	LYS

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Mol	Chain	Res	Type
1	B	254	LEU
1	B	265	GLU
1	B	280	GLU
1	B	293	ASN
1	B	342	MET
1	B	349	ASP
1	B	398	ILE
1	B	435	LEU
1	B	451	VAL
1	B	456	ARG
1	B	457	ARG
1	B	458	THR
1	B	461	ASP
1	B	472	ARG
1	B	473	LEU
1	B	483	ASN
1	B	508	ARG
1	B	528	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	40	GLN
1	A	70	HIS
1	A	80	ASN
1	A	119	GLN
1	A	139	ASN
1	A	147	GLN
1	A	163	ASN
1	A	230	HIS
1	A	231	ASN
1	A	299	HIS
1	A	385	GLN
1	A	448	GLN
1	A	455	HIS
1	A	483	ASN
1	A	505	HIS
1	A	512	GLN
1	A	527	ASN
1	B	30	HIS
1	B	40	GLN

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Mol	Chain	Res	Type
1	B	70	HIS
1	B	74	ASN
1	B	139	ASN
1	B	147	GLN
1	B	163	ASN
1	B	231	ASN
1	B	293	ASN
1	B	299	HIS
1	B	339	ASN
1	B	441	GLN
1	B	455	HIS
1	B	483	ASN
1	B	505	HIS
1	B	512	GLN
1	B	527	ASN

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
3	SO4	B	531	-	4,4,4	0.32	0	6,6,6	0.14	0
3	SO4	A	531	-	4,4,4	0.36	0	6,6,6	0.16	0
2	BTN	A	5600	-	17,17,17	3.77	8 (47%)	23,23,23	2.79	7 (30%)
2	BTN	B	5601	-	17,17,17	3.44	7 (41%)	23,23,23	2.96	7 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BTN	A	5600	-	-	4/7/28/28	0/2/2/2
2	BTN	B	5601	-	-	4/7/28/28	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5600	BTN	C5-N1	8.23	1.58	1.46
2	B	5601	BTN	C5-N1	6.94	1.56	1.46
2	A	5600	BTN	C2-S1	6.80	1.93	1.82
2	B	5601	BTN	C2-S1	6.62	1.93	1.82
2	A	5600	BTN	C3-N2	6.06	1.46	1.35
2	A	5600	BTN	C4-N2	5.59	1.56	1.45
2	B	5601	BTN	C3-N2	5.35	1.45	1.35
2	B	5601	BTN	C4-N2	5.18	1.55	1.45
2	A	5600	BTN	C3-N1	-4.48	1.27	1.35
2	B	5601	BTN	C3-N1	-4.32	1.27	1.35
2	A	5600	BTN	C6-S1	4.09	1.92	1.81
2	B	5601	BTN	C6-S1	3.96	1.92	1.81
2	A	5600	BTN	O3-C3	3.28	1.30	1.23
2	B	5601	BTN	O3-C3	2.67	1.29	1.23
2	A	5600	BTN	O12-C11	-2.07	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5601	BTN	O3-C3-N2	-7.67	114.86	125.89
2	A	5600	BTN	O3-C3-N2	-6.68	116.28	125.89
2	B	5601	BTN	C4-N2-C3	-6.05	105.05	112.56
2	A	5600	BTN	C4-N2-C3	-5.77	105.39	112.56
2	A	5600	BTN	C6-C5-N1	-5.50	106.10	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5601	BTN	C6-C5-N1	-5.43	106.19	113.18
2	B	5601	BTN	N2-C3-N1	4.28	113.80	108.85
2	B	5601	BTN	C6-C5-C4	3.83	115.14	109.06
2	B	5601	BTN	O3-C3-N1	3.78	131.34	125.89
2	A	5600	BTN	C6-C5-C4	3.77	115.03	109.06
2	A	5600	BTN	N2-C3-N1	3.71	113.13	108.85
2	A	5600	BTN	C5-C4-N2	3.60	106.74	102.68
2	B	5601	BTN	C5-C4-N2	3.51	106.64	102.68
2	A	5600	BTN	O3-C3-N1	3.26	130.59	125.89

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5600	BTN	C7-C8-C9-C10
2	B	5601	BTN	C11-C10-C9-C8
2	A	5600	BTN	C11-C10-C9-C8
2	B	5601	BTN	C7-C8-C9-C10
2	B	5601	BTN	C9-C10-C11-O12
2	B	5601	BTN	C9-C10-C11-O11
2	A	5600	BTN	C9-C10-C11-O12
2	A	5600	BTN	C9-C10-C11-O11

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5600	BTN	2	0
2	B	5601	BTN	2	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 [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	521/530 (98%)	-1.29	0 100 100	22, 30, 54, 113	0
1	B	521/530 (98%)	-1.28	0 100 100	22, 31, 56, 102	0
All	All	1042/1060 (98%)	-1.28	0 100 100	22, 30, 56, 113	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	BTN	A	5600	16/16	0.98	0.07	54,57,69,70	0
2	BTN	B	5601	16/16	0.98	0.06	55,58,75,75	0
3	SO4	B	531	5/5	0.99	0.04	36,38,39,40	0
3	SO4	A	531	5/5	1.00	0.02	38,38,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.