Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 11:08 PM EDT

PDB ID	:	1PWQ
Title	:	Crystal structure of Anthrax Lethal Factor complexed with Thioacetyl-Tyr-Pro-Met-Amide, a metal-chelating peptidyl small molecule inhibitor
Authors	:	Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on	:	2003-07-02
Resolution	:	3.52 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:

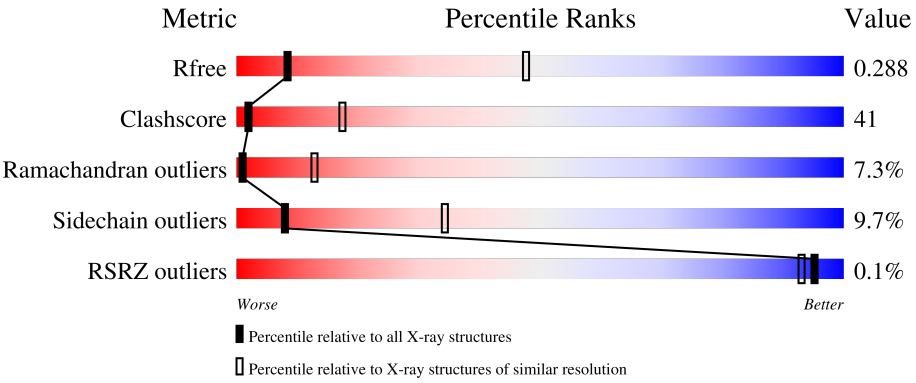
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 <=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	776	31% 54% 9% 6%
1	B	776	33% 52% 9% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12120 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.

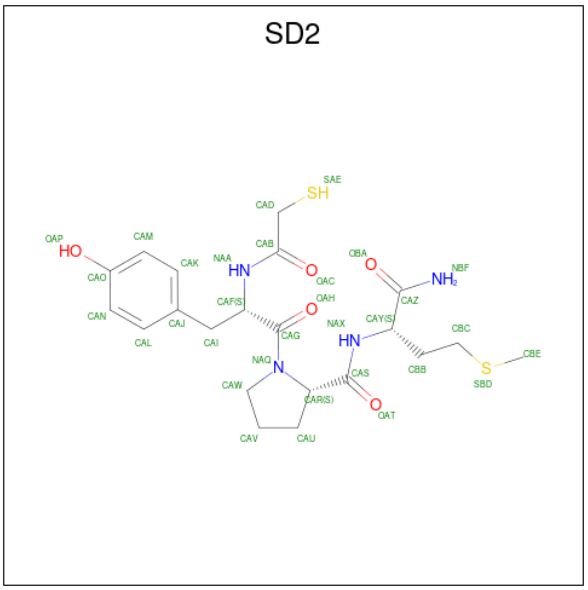
- Molecule 1 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			6020	3827	1015	1171	7			
1	B	734	Total	C	N	O	S	0	0	0
			6034	3834	1017	1176	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-(SULFANYLACETYL)TYROSYLPROLYLMETHIONINAMIDE (three-letter code: SD2) (formula: $C_{21}H_{30}N_4O_5S_2$).



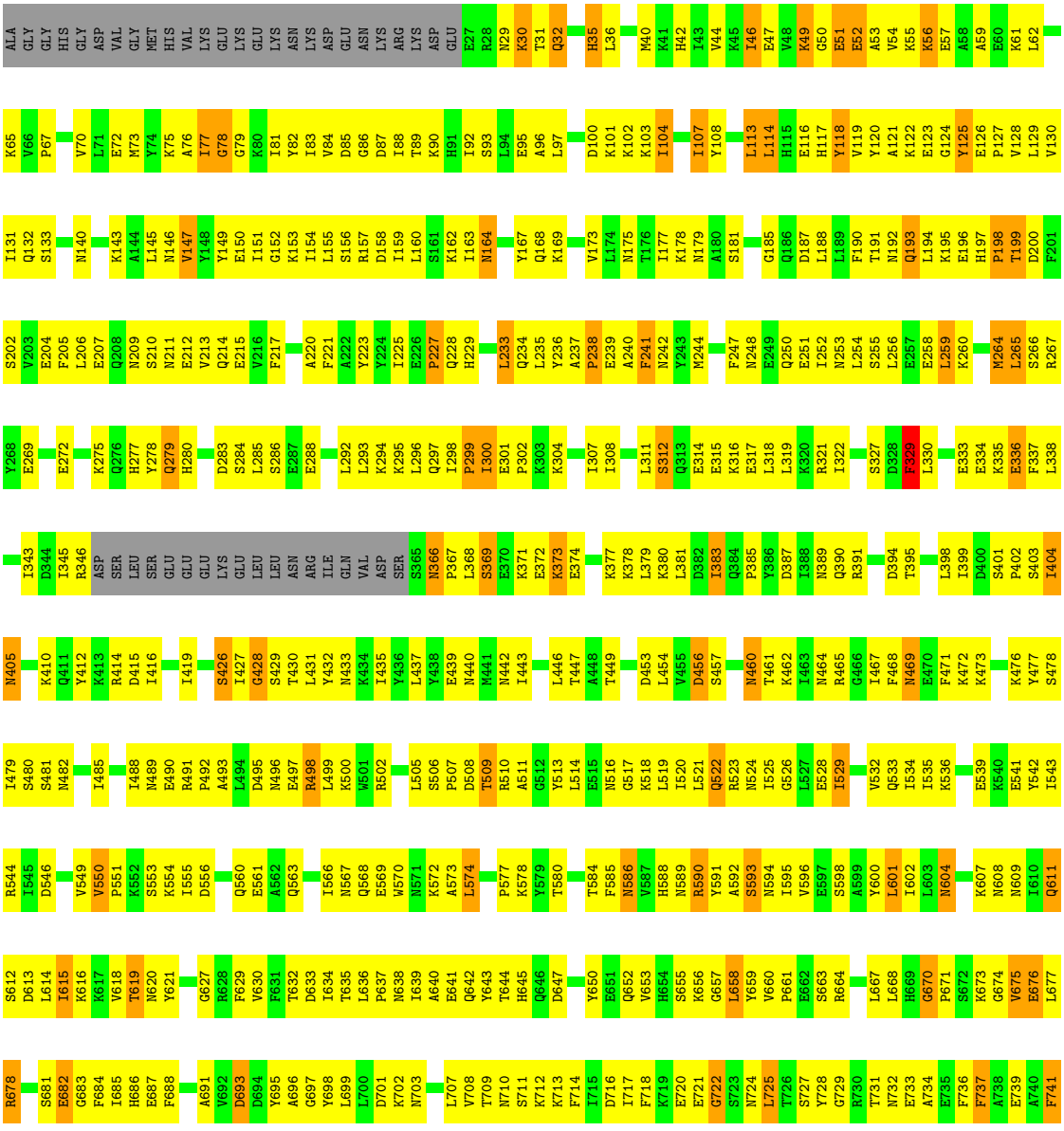
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	21	4	5	2		
3	B	1	Total	C	N	O	S	0	0
			32	21	4	5	2		

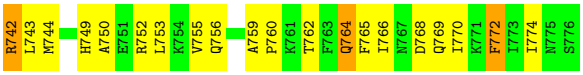
3 Residue-property plots (i)

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: Lethal factor

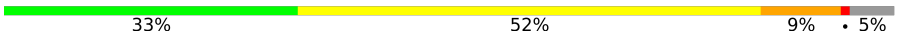
Chain A:

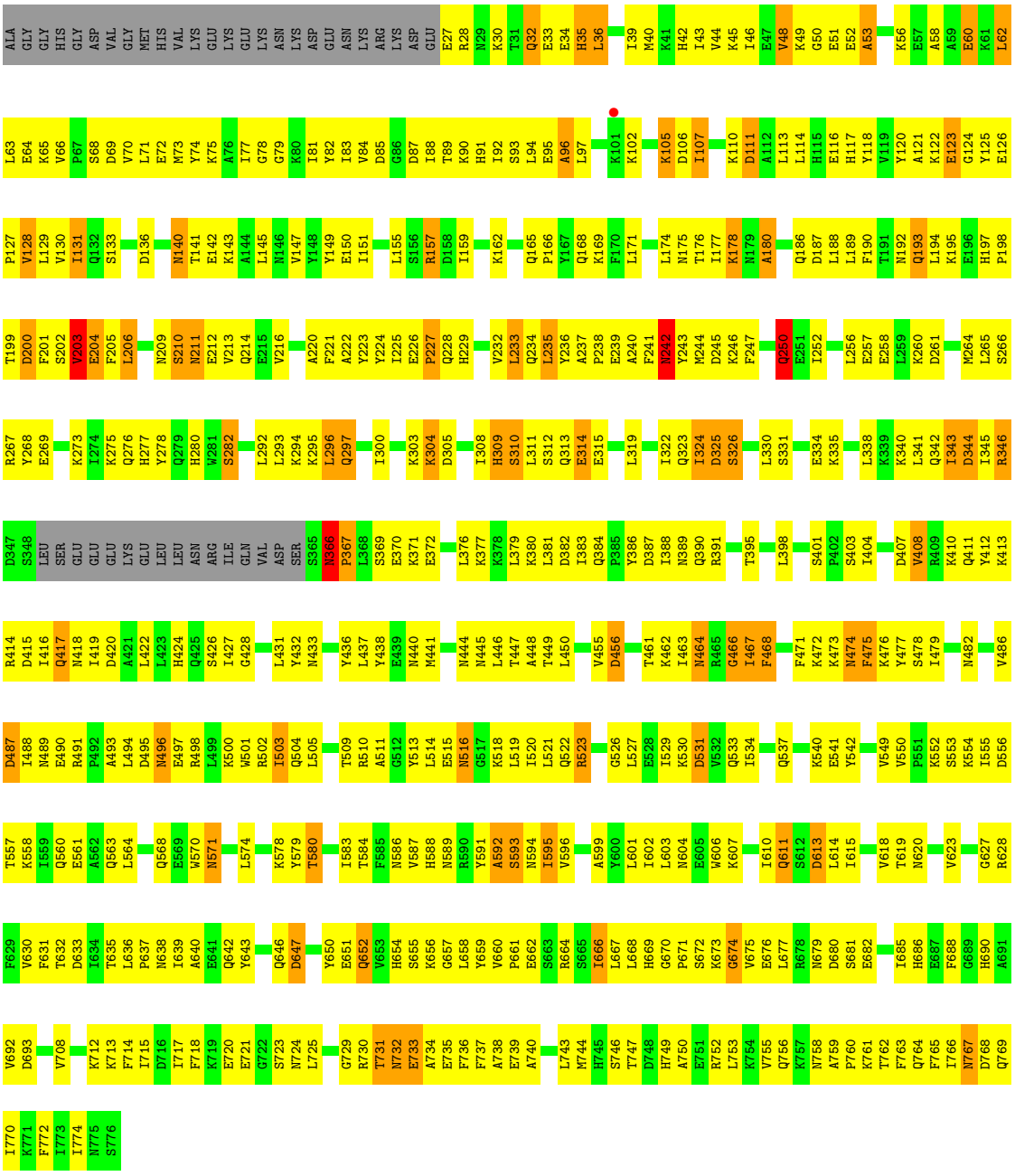




• Molecule 1: Lethal factor

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	24.86 – 3.52 24.86 – 3.51	Depositor EDS
% Data completeness (in resolution range)	86.7 (24.86-3.52) 82.4 (24.86-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 3.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.311 0.208 , 0.288	Depositor DCC
R_{free} test set	1331 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , -3.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.066 for l,-k,h	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12120	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SD2, ZN

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	0.48	0/6128	0.70	0/8253
1	B	0.50	0/6142	0.72	0/8272
All	All	0.49	0/12270	0.71	0/16525

There are no bond length outliers.

There are no bond angle outliers.

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	6020	0	6008	498	0
1	B	6034	0	6017	501	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	28	9	0
3	B	32	0	29	9	0
All	All	12120	0	12082	1000	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 41.

All (1000) 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:91:HIS:CD2	1:B:93:SER:HB3	1.69	1.27
1:A:635:THR:HG22	1:A:637:PRO:HD2	1.21	1.16
1:B:366:ASN:HB2	1:B:367:PRO:HD3	1.16	1.12
1:A:308:ILE:HD12	1:A:345:ILE:HD11	1.32	1.10
1:B:91:HIS:HD2	1:B:93:SER:HB3	0.92	1.09
1:B:91:HIS:CD2	1:B:93:SER:CB	2.38	1.07
1:A:49:LYS:HG3	1:A:50:GLY:H	1.24	1.02
1:B:340:LYS:O	1:B:344:ASP:OD1	1.81	0.99
1:B:366:ASN:CB	1:B:367:PRO:HD3	1.92	0.98
1:A:440:ASN:HD21	1:A:500:LYS:HE2	1.29	0.98
1:B:175:ASN:ND2	1:B:200:ASP:HB3	1.81	0.96
1:B:366:ASN:HB2	1:B:367:PRO:CD	1.89	0.96
1:B:175:ASN:HD21	1:B:200:ASP:HB3	1.28	0.95
1:A:304:LYS:H	1:A:304:LYS:HD2	1.31	0.95
1:B:165:GLN:HG3	1:B:166:PRO:HA	1.48	0.95
1:A:477:TYR:H	1:A:593:SER:HB2	1.30	0.94
1:B:296:LEU:HD22	1:B:419:ILE:HD13	1.48	0.94
1:A:426:SER:HA	1:A:510:ARG:HA	1.50	0.93
1:B:273:LYS:HD2	1:B:431:LEU:HD22	1.53	0.91
1:A:31:THR:O	1:A:35:HIS:HB3	1.70	0.91
1:A:643:TYR:HB3	1:A:652:GLN:OE1	1.72	0.90
3:B:9003:SD2:OAT	3:B:9003:SD2:HAL	1.74	0.88
1:A:500:LYS:HZ2	1:A:500:LYS:HB3	1.36	0.88
1:A:301:GLU:HG3	1:A:385:PRO:HG3	1.56	0.88
1:A:373:LYS:HG2	1:A:377:LYS:HE3	1.54	0.87
1:A:655:SER:HB2	3:A:9002:SD2:OAH	1.75	0.86
1:A:173:VAL:O	1:A:177:ILE:HG12	1.75	0.86
1:B:221:PHE:HA	1:B:244:MET:HE2	1.57	0.86
1:A:40:MET:O	1:A:44:VAL:HB	1.76	0.85
1:B:686:HIS:ND1	3:B:9003:SD2:HAK	1.92	0.85
1:A:412:TYR:O	1:A:416:ILE:HG13	1.77	0.85
1:B:516:ASN:H	1:B:516:ASN:HD22	1.23	0.84
1:B:366:ASN:HD22	1:B:367:PRO:CD	1.90	0.84
1:B:516:ASN:HD22	1:B:516:ASN:N	1.75	0.84
1:A:308:ILE:HD12	1:A:345:ILE:CD1	2.06	0.84
1:A:469:ASN:N	1:A:469:ASN:HD22	1.74	0.84
1:B:140:ASN:C	1:B:140:ASN:HD22	1.79	0.83
1:A:442:ASN:HB2	1:A:496:ASN:HD22	1.44	0.82
1:A:59:ALA:HB1	1:A:83:ILE:HD13	1.62	0.82
1:B:516:ASN:H	1:B:516:ASN:ND2	1.75	0.82
1:B:91:HIS:CD2	1:B:93:SER:H	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:PHE:CZ	1:B:534:ILE:HG13	2.16	0.81
1:B:36:LEU:HD13	1:B:64:GLU:OE1	1.80	0.81
1:A:440:ASN:ND2	1:A:500:LYS:HE2	1.96	0.81
1:A:167:TYR:CZ	1:A:536:LYS:HB2	2.16	0.80
1:A:308:ILE:CD1	1:A:345:ILE:HD11	2.11	0.80
1:A:102:LYS:HA	1:A:114:LEU:HD11	1.61	0.80
1:A:490:GLU:OE2	1:A:544:ARG:NH2	2.12	0.80
1:A:608:ASN:C	1:A:609:ASN:HD22	1.85	0.79
1:B:81:ILE:HG23	1:B:129:LEU:HD22	1.65	0.79
1:B:113:LEU:O	1:B:116:GLU:HG2	1.83	0.79
1:B:557:THR:O	1:B:561:GLU:HG3	1.82	0.78
1:B:570:TRP:CE3	1:B:574:LEU:HD21	2.17	0.78
1:B:401:SER:CB	1:B:638:ASN:HD22	1.96	0.77
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.50	0.77
1:B:186:GLN:HE21	1:B:195:LYS:HB2	1.50	0.77
1:B:75:LYS:O	1:B:78:GLY:N	2.16	0.76
1:B:304:LYS:HD3	1:B:304:LYS:H	1.47	0.76
1:B:611:GLN:HE21	1:B:774:ILE:CD1	1.99	0.76
1:A:167:TYR:CE1	1:A:536:LYS:HB2	2.21	0.76
1:B:224:TYR:HD2	1:B:225:ILE:HD13	1.51	0.76
1:B:324:ILE:O	1:B:326:SER:N	2.18	0.76
1:A:233:LEU:O	1:A:237:ALA:HB3	1.85	0.76
1:A:518:LYS:O	1:A:519:LEU:HD23	1.86	0.75
1:A:676:GLU:O	1:A:677:LEU:HD23	1.85	0.75
1:B:463:ILE:HD12	1:B:534:ILE:HG23	1.68	0.75
1:A:61:LYS:HA	1:A:61:LYS:HE2	1.69	0.75
1:A:764:GLN:O	1:A:768:ASP:HB2	1.87	0.75
1:A:73:MET:HG2	1:A:256:LEU:HD23	1.69	0.75
1:A:87:ASP:HB3	1:A:90:LYS:HE3	1.69	0.74
1:B:343:ILE:HD13	1:B:343:ILE:N	2.02	0.74
1:A:87:ASP:O	1:A:90:LYS:HG2	1.87	0.74
1:A:49:LYS:HG3	1:A:50:GLY:N	1.97	0.74
1:B:635:THR:HB	1:B:637:PRO:HD2	1.69	0.74
1:A:709:THR:HG21	1:A:734:ALA:HA	1.67	0.74
1:B:366:ASN:HD22	1:B:367:PRO:HD3	1.50	0.74
1:A:500:LYS:HB3	1:A:500:LYS:NZ	2.02	0.74
1:A:389:ASN:OD1	1:A:482:ASN:HB2	1.88	0.74
1:B:401:SER:HB2	1:B:638:ASN:HD22	1.51	0.73
1:A:658:LEU:HD23	3:A:9002:SD2:SAE	2.28	0.73
1:B:708:VAL:HG21	1:B:769:GLN:NE2	2.03	0.73
1:B:610:ILE:HD12	1:B:610:ILE:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:GLN:HE21	1:A:774:ILE:HD11	1.54	0.72
1:A:258:GLU:HG3	1:A:502:ARG:HH12	1.54	0.72
1:B:211:ASN:HA	1:B:214:GLN:NE2	2.04	0.72
1:A:613:ASP:HB3	1:A:774:ILE:HG23	1.72	0.71
1:B:145:LEU:HD23	1:B:226:GLU:HG3	1.72	0.71
1:A:677:LEU:HD11	3:A:9002:SD2:CAO	2.20	0.71
1:B:343:ILE:O	1:B:346:ARG:HB2	1.90	0.71
1:B:688:PHE:O	1:B:692:VAL:HG23	1.90	0.70
1:A:298:ILE:O	1:A:298:ILE:HD12	1.91	0.70
1:B:88:ILE:HB	1:B:130:VAL:HG11	1.73	0.70
1:B:583:ILE:HG23	1:B:631:PHE:HE1	1.56	0.70
1:B:123:GLU:HG3	1:B:157:ARG:NH1	2.06	0.70
1:A:202:SER:O	1:A:205:PHE:N	2.25	0.70
1:A:107:ILE:HG23	1:A:108:TYR:H	1.57	0.70
1:B:570:TRP:HE3	1:B:574:LEU:HD21	1.55	0.70
1:B:646:GLN:NE2	1:B:652:GLN:HB3	2.07	0.70
1:A:95:GLU:HG3	1:A:95:GLU:O	1.91	0.70
1:A:107:ILE:HG23	1:A:108:TYR:N	2.06	0.70
1:B:630:VAL:HB	1:B:667:LEU:HD23	1.74	0.70
1:A:113:LEU:O	1:A:117:HIS:HB2	1.91	0.69
1:A:567:ASN:C	1:A:569:GLU:H	1.96	0.69
1:B:366:ASN:CB	1:B:367:PRO:CD	2.58	0.69
1:B:27:GLU:HG3	1:B:27:GLU:O	1.92	0.69
1:A:693:ASP:OD2	1:A:707:LEU:HB2	1.93	0.69
1:A:500:LYS:HZ2	1:A:544:ARG:HH21	1.40	0.69
1:B:111:ASP:N	1:B:111:ASP:OD2	2.26	0.69
1:B:461:THR:HG22	1:B:540:LYS:HA	1.74	0.69
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.57	0.69
1:A:513:TYR:HA	1:A:519:LEU:CD2	2.23	0.69
1:B:70:VAL:HG13	1:B:155:LEU:HD13	1.74	0.68
1:B:278:TYR:HE2	1:B:511:ALA:O	1.76	0.68
1:B:675:VAL:HG23	3:B:9003:SD2:CAZ	2.24	0.68
1:A:513:TYR:HA	1:A:519:LEU:HD22	1.74	0.68
1:B:114:LEU:HA	1:B:117:HIS:HB3	1.75	0.68
1:B:300:ILE:O	1:B:300:ILE:HG22	1.93	0.68
1:B:233:LEU:HD23	1:B:237:ALA:HB3	1.75	0.68
1:A:395:THR:HB	1:A:398:LEU:O	1.93	0.68
1:A:442:ASN:ND2	1:A:496:ASN:HB2	2.09	0.68
1:B:107:ILE:HG21	1:B:145:LEU:HD12	1.75	0.68
1:B:246:LYS:O	1:B:250:GLN:HB2	1.94	0.68
1:B:610:ILE:CG2	1:B:614:LEU:HD23	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:O	1:A:285:LEU:HD23	1.95	0.67
1:A:498:ARG:HD3	1:A:542:TYR:CD2	2.30	0.67
1:A:585:PHE:CE1	1:A:596:VAL:HG13	2.30	0.67
1:B:129:LEU:HD21	1:B:131:ILE:HG12	1.75	0.67
1:B:603:LEU:O	1:B:606:TRP:HB3	1.93	0.67
1:A:103:LYS:HG3	1:A:113:LEU:HD21	1.77	0.67
1:A:577:PRO:O	1:A:580:THR:HG22	1.95	0.67
1:A:191:THR:HG23	1:A:193:GLN:H	1.60	0.67
1:A:369:SER:OG	1:A:372:GLU:HB2	1.93	0.67
1:B:366:ASN:ND2	1:B:367:PRO:HD3	2.09	0.67
1:B:746:SER:O	1:B:752:ARG:HD2	1.94	0.67
1:B:126:GLU:N	1:B:127:PRO:HD3	2.10	0.66
1:B:140:ASN:HD22	1:B:141:THR:N	1.93	0.66
1:A:102:LYS:HA	1:A:114:LEU:CD1	2.25	0.66
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.30	0.66
1:B:475:PHE:CD1	1:B:529:ILE:HG12	2.30	0.66
1:B:516:ASN:N	1:B:516:ASN:ND2	2.40	0.66
1:B:107:ILE:HD13	1:B:107:ILE:O	1.96	0.66
1:B:386:TYR:OH	1:B:411:GLN:HG3	1.95	0.66
1:B:643:TYR:HA	1:B:646:GLN:HB2	1.77	0.66
1:B:755:VAL:HG12	1:B:763:PHE:HB2	1.78	0.66
1:A:296:LEU:HD12	1:A:419:ILE:HD13	1.78	0.65
1:B:477:TYR:H	1:B:593:SER:HB2	1.62	0.65
1:A:427:ILE:HG23	1:A:428:GLY:N	2.09	0.65
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.11	0.65
1:B:438:TYR:CE2	1:B:502:ARG:HD3	2.32	0.65
1:B:212:GLU:O	1:B:216:VAL:HG23	1.96	0.65
1:A:500:LYS:HZ2	1:A:544:ARG:NH2	1.94	0.65
1:A:314:GLU:HA	1:A:317:GLU:CD	2.17	0.65
1:A:334:GLU:O	1:A:337:PHE:HB3	1.96	0.65
1:B:627:GLY:O	1:B:628:ARG:HG2	1.96	0.65
1:B:655:SER:HB2	3:B:9003:SD2:OAH	1.96	0.65
1:B:377:LYS:O	1:B:380:LYS:HB3	1.97	0.64
1:B:74:TYR:HA	1:B:159:ILE:HD11	1.79	0.64
1:B:366:ASN:HD22	1:B:367:PRO:HD2	1.62	0.64
1:A:59:ALA:CB	1:A:83:ILE:HD13	2.27	0.64
1:B:49:LYS:HG3	1:B:85:ASP:HB3	1.80	0.64
1:B:670:GLY:H	1:B:671:PRO:HD3	1.63	0.64
1:B:36:LEU:O	1:B:40:MET:HG3	1.98	0.64
1:A:304:LYS:H	1:A:304:LYS:CD	2.08	0.64
1:A:485:ILE:HG12	1:A:520:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:O	1:A:154:ILE:HB	1.99	0.63
1:A:394:ASP:O	1:A:634:ILE:HB	1.98	0.63
1:A:427:ILE:CG2	1:A:428:GLY:N	2.61	0.63
1:A:252:ILE:HG23	1:A:253:ASN:N	2.13	0.63
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.61	0.63
1:A:329:PHE:N	1:A:329:PHE:HD2	1.97	0.63
1:A:498:ARG:HD3	1:A:542:TYR:CE2	2.34	0.63
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.81	0.63
1:A:673:LYS:O	3:A:9002:SD2:HAY	1.99	0.63
1:B:686:HIS:CE1	3:B:9003:SD2:HAK	2.34	0.63
1:A:36:LEU:O	1:A:40:MET:HG2	1.99	0.63
1:B:45:LYS:HD2	1:B:82:TYR:CE2	2.33	0.63
1:B:650:TYR:CE1	1:B:651:GLU:HG3	2.33	0.63
1:A:73:MET:HB3	1:A:159:ILE:HD13	1.81	0.62
1:A:550:VAL:HG12	1:A:551:PRO:HD2	1.81	0.62
1:B:257:GLU:O	1:B:260:LYS:HB2	1.99	0.62
1:A:119:VAL:HG13	1:A:131:ILE:HG12	1.81	0.62
1:B:552:LYS:O	1:B:554:LYS:N	2.33	0.62
1:B:456:ASP:HB3	1:B:462:LYS:O	1.98	0.62
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.34	0.62
1:B:493:ALA:HB1	1:B:497:GLU:HB2	1.81	0.62
1:B:494:LEU:O	1:B:496:ASN:N	2.31	0.62
1:B:723:SER:HA	1:B:730:ARG:HD3	1.81	0.62
1:A:107:ILE:C	1:A:107:ILE:HD13	2.19	0.62
1:A:126:GLU:O	1:A:128:VAL:HG23	1.99	0.62
1:A:477:TYR:N	1:A:593:SER:HB2	2.10	0.62
1:B:232:VAL:O	1:B:235:LEU:HD12	2.00	0.62
1:B:43:ILE:HG13	1:B:44:VAL:HG23	1.81	0.62
1:B:366:ASN:ND2	1:B:367:PRO:CD	2.61	0.62
1:B:570:TRP:HH2	1:B:607:LYS:HB2	1.65	0.62
1:A:635:THR:HG22	1:A:637:PRO:CD	2.14	0.62
1:B:574:LEU:N	1:B:574:LEU:HD23	2.15	0.62
1:A:329:PHE:HD2	1:A:329:PHE:H	1.46	0.61
1:A:256:LEU:HD11	1:A:260:LYS:HE3	1.81	0.61
1:A:707:LEU:HD12	1:A:709:THR:CG2	2.30	0.61
1:B:105:LYS:HD2	1:B:105:LYS:N	2.15	0.61
1:A:221:PHE:O	1:A:225:ILE:HG12	2.00	0.61
1:B:240:ALA:O	1:B:244:MET:HB2	2.00	0.61
1:B:503:ILE:HD13	1:B:503:ILE:N	2.15	0.61
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.82	0.61
1:B:650:TYR:CD1	1:B:651:GLU:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LYS:C	1:A:337:PHE:H	2.02	0.61
1:A:296:LEU:C	1:A:296:LEU:HD23	2.20	0.61
1:B:686:HIS:HD2	1:B:738:ALA:HB1	1.66	0.61
1:B:725:LEU:HD12	1:B:736:PHE:CE1	2.36	0.61
1:A:67:PRO:O	1:A:70:VAL:HG22	2.01	0.61
1:B:73:MET:HG2	1:B:256:LEU:HD12	1.83	0.61
1:B:733:GLU:CD	1:B:733:GLU:H	2.03	0.61
1:A:30:LYS:O	1:A:30:LYS:HG3	1.99	0.61
1:B:540:LYS:HD3	1:B:542:TYR:OH	2.00	0.61
1:A:102:LYS:O	1:A:114:LEU:HG	2.01	0.60
1:A:319:LEU:HA	1:A:322:ILE:HD12	1.81	0.60
1:B:125:TYR:C	1:B:127:PRO:HD3	2.21	0.60
1:B:131:ILE:HD11	1:B:147:VAL:CG1	2.30	0.60
1:B:242:ASN:O	1:B:243:TYR:C	2.39	0.60
1:B:292:LEU:HD11	1:B:418:ASN:HB3	1.82	0.60
1:B:673:LYS:O	1:B:673:LYS:HG3	2.01	0.60
1:B:708:VAL:HG21	1:B:769:GLN:HE22	1.67	0.60
1:A:175:ASN:OD1	1:A:200:ASP:HB3	2.01	0.60
1:A:635:THR:CG2	1:A:637:PRO:HD2	2.14	0.60
1:A:469:ASN:N	1:A:469:ASN:ND2	2.45	0.60
1:A:543:ILE:HG22	1:A:543:ILE:O	2.01	0.60
1:A:76:ALA:C	1:A:78:GLY:H	2.04	0.60
1:A:258:GLU:HG3	1:A:502:ARG:NH1	2.15	0.60
1:A:637:PRO:HG3	1:A:653:VAL:O	2.02	0.60
1:A:329:PHE:N	1:A:329:PHE:CD2	2.69	0.60
1:B:513:TYR:O	1:B:514:LEU:HD23	2.01	0.60
1:A:191:THR:HG22	1:A:194:LEU:HG	1.83	0.60
1:B:210:SER:O	1:B:212:GLU:N	2.35	0.60
1:B:447:THR:HG21	1:B:450:LEU:HD12	1.84	0.60
1:A:766:ILE:O	1:A:770:ILE:HG12	2.02	0.59
1:B:440:ASN:ND2	1:B:500:LYS:HD3	2.17	0.59
1:A:476:LYS:H	1:A:593:SER:CB	2.13	0.59
1:A:301:GLU:HG3	1:A:385:PRO:CG	2.30	0.59
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.82	0.59
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.85	0.59
1:A:338:LEU:HD21	1:A:383:ILE:HG21	1.84	0.59
1:B:83:ILE:HG23	1:B:131:ILE:HG22	1.83	0.59
1:B:245:ASP:C	1:B:245:ASP:OD2	2.41	0.59
1:A:608:ASN:N	1:A:608:ASN:HD22	1.99	0.59
1:B:202:SER:O	1:B:204:GLU:N	2.35	0.59
1:B:557:THR:O	1:B:560:GLN:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:HD21	1:A:380:LYS:HB2	1.83	0.59
1:A:454:LEU:HA	1:A:467:ILE:HG21	1.85	0.59
1:B:666:ILE:HG22	1:B:667:LEU:N	2.18	0.59
1:A:739:GLU:O	1:A:743:LEU:HD12	2.03	0.59
1:B:413:LYS:O	1:B:417:GLN:HG3	2.03	0.59
1:A:464:ASN:OD1	1:A:467:ILE:HD13	2.03	0.58
1:B:636:LEU:N	1:B:636:LEU:HD12	2.16	0.58
1:A:241:PHE:CD1	1:A:241:PHE:C	2.76	0.58
1:A:307:ILE:O	1:A:311:LEU:HD13	2.02	0.58
1:B:619:THR:O	1:B:623:VAL:HG23	2.03	0.58
1:B:656:LYS:HD3	1:B:672:SER:HB3	1.83	0.58
1:A:601:LEU:HD23	1:A:601:LEU:H	1.68	0.58
1:B:221:PHE:O	1:B:225:ILE:HG12	2.04	0.58
1:B:401:SER:HB2	1:B:638:ASN:ND2	2.18	0.58
1:A:73:MET:CG	1:A:256:LEU:HD23	2.34	0.58
1:A:267:ARG:O	1:A:489:ASN:ND2	2.36	0.58
1:B:477:TYR:HB2	1:B:555:ILE:HD13	1.86	0.58
1:B:202:SER:OG	1:B:204:GLU:HG3	2.03	0.58
1:B:221:PHE:CD1	1:B:244:MET:HE1	2.35	0.58
1:B:686:HIS:CD2	1:B:738:ALA:HB1	2.39	0.58
1:A:677:LEU:HD21	3:A:9002:SD2:OAP	2.02	0.58
1:A:461:THR:O	1:A:541:GLU:HB2	2.04	0.58
1:B:69:ASP:O	1:B:73:MET:HG3	2.04	0.57
1:B:155:LEU:O	1:B:159:ILE:HB	2.03	0.57
1:B:338:LEU:O	1:B:341:LEU:HB3	2.03	0.57
1:B:496:ASN:HD22	1:B:497:GLU:N	2.02	0.57
1:A:368:LEU:O	1:A:369:SER:HB3	2.04	0.57
1:B:444:ASN:OD1	1:B:448:ALA:HA	2.04	0.57
1:A:338:LEU:HD22	1:A:379:LEU:HD13	1.85	0.57
3:A:9002:SD2:HAL	3:A:9002:SD2:OAT	2.04	0.57
1:B:224:TYR:CD2	1:B:225:ILE:HD13	2.37	0.57
1:B:571:ASN:HD21	1:B:580:THR:HG22	1.68	0.57
1:B:236:TYR:C	1:B:238:PRO:HD3	2.24	0.57
1:B:510:ARG:O	1:B:522:GLN:HB3	2.04	0.57
1:A:202:SER:O	1:A:205:PHE:HB3	2.04	0.57
1:B:84:VAL:O	1:B:133:SER:N	2.31	0.57
1:B:140:ASN:C	1:B:140:ASN:ND2	2.50	0.57
1:B:330:LEU:O	1:B:335:LYS:HE3	2.03	0.57
1:B:91:HIS:CD2	1:B:93:SER:N	2.71	0.57
1:B:555:ILE:O	1:B:558:LYS:HB2	2.05	0.57
1:A:122:LYS:N	1:A:128:VAL:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LEU:HD23	1:A:601:LEU:N	2.20	0.57
1:A:602:ILE:HG23	1:A:681:SER:HA	1.87	0.57
1:A:762:THR:HG22	1:A:766:ILE:HD13	1.87	0.57
1:B:468:PHE:CE1	1:B:534:ILE:CG1	2.87	0.57
1:B:221:PHE:HD1	1:B:244:MET:CE	2.16	0.57
1:B:257:GLU:O	1:B:260:LYS:N	2.38	0.56
1:B:438:TYR:HE2	1:B:502:ARG:HD3	1.70	0.56
1:A:674:GLY:O	1:A:676:GLU:N	2.38	0.56
1:B:714:PHE:HE2	1:B:733:GLU:HB2	1.70	0.56
1:B:611:GLN:HE21	1:B:774:ILE:HD11	1.70	0.56
1:A:391:ARG:NH2	1:A:399:ILE:O	2.38	0.56
1:A:643:TYR:CB	1:A:652:GLN:OE1	2.48	0.56
1:B:94:LEU:O	1:B:96:ALA:N	2.38	0.56
1:B:105:LYS:HE2	1:B:111:ASP:HB3	1.87	0.56
1:B:404:ILE:HD12	1:B:408:VAL:HB	1.87	0.56
1:A:167:TYR:CE1	1:A:536:LYS:CB	2.88	0.56
1:B:221:PHE:CE1	1:B:225:ILE:HD11	2.41	0.56
1:B:403:SER:OG	1:B:638:ASN:ND2	2.39	0.56
1:A:598:SER:O	1:A:602:ILE:HG13	2.05	0.56
1:B:438:TYR:O	1:B:486:VAL:HB	2.06	0.56
1:B:583:ILE:HG23	1:B:631:PHE:CE1	2.39	0.56
1:B:656:LYS:CD	1:B:672:SER:HB3	2.36	0.56
1:A:737:PHE:HD2	1:A:737:PHE:C	2.09	0.56
1:B:131:ILE:HD11	1:B:147:VAL:HG13	1.86	0.56
1:B:68:SER:O	1:B:71:LEU:N	2.39	0.56
1:B:91:HIS:CD2	1:B:93:SER:HB2	2.37	0.56
1:A:737:PHE:C	1:A:737:PHE:CD2	2.80	0.55
1:A:253:ASN:O	1:A:255:SER:N	2.40	0.55
1:A:506:SER:OG	1:A:508:ASP:HB2	2.06	0.55
1:A:658:LEU:HD22	1:A:659:TYR:N	2.21	0.55
1:B:427:ILE:HG23	1:B:428:GLY:N	2.21	0.55
1:B:117:HIS:CG	1:B:118:TYR:H	2.24	0.55
1:B:127:PRO:O	1:B:128:VAL:HG13	2.07	0.55
1:A:123:GLU:O	1:A:123:GLU:HG3	2.05	0.55
1:A:639:ILE:HG21	1:A:667:LEU:CD2	2.36	0.55
1:A:681:SER:O	1:A:682:GLU:C	2.44	0.55
1:B:280:HIS:C	1:B:282:SER:H	2.10	0.55
1:B:602:ILE:HD13	1:B:668:LEU:HD21	1.87	0.55
1:B:766:ILE:C	1:B:768:ASP:H	2.10	0.55
1:A:107:ILE:CG2	1:A:108:TYR:H	2.18	0.55
1:A:525:ILE:HG22	1:A:526:GLY:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:HIS:O	1:B:39:ILE:HG12	2.06	0.55
1:B:713:LYS:HD2	1:B:765:PHE:HE1	1.72	0.55
1:B:319:LEU:HD23	1:B:345:ILE:HD11	1.89	0.55
1:A:304:LYS:HD2	1:A:304:LYS:N	2.12	0.55
1:A:477:TYR:CE1	1:A:593:SER:HA	2.40	0.55
1:A:642:GLN:OE1	1:A:653:VAL:HG22	2.07	0.55
1:A:206:LEU:O	1:A:210:SER:HB3	2.07	0.54
1:A:769:GLN:O	1:A:772:PHE:HB3	2.07	0.54
1:B:32:GLN:O	1:B:34:GLU:N	2.39	0.54
1:B:431:LEU:O	1:B:432:TYR:HB3	2.08	0.54
1:B:714:PHE:HA	1:B:717:ILE:HG12	1.89	0.54
1:A:122:LYS:HB3	1:A:128:VAL:HB	1.89	0.54
1:A:762:THR:CG2	1:A:766:ILE:HD13	2.37	0.54
1:B:210:SER:O	1:B:211:ASN:C	2.44	0.54
1:B:303:LYS:HD2	1:B:305:ASP:OD1	2.06	0.54
1:B:369:SER:OG	1:B:372:GLU:HG3	2.07	0.54
1:A:49:LYS:CG	1:A:50:GLY:N	2.69	0.54
1:A:250:GLN:HG3	1:A:251:GLU:HG2	1.90	0.54
1:A:387:ASP:HB3	1:A:390:GLN:HB3	1.90	0.54
1:A:247:PHE:CZ	1:A:252:ILE:HD12	2.42	0.54
1:B:83:ILE:HD12	1:B:131:ILE:HG21	1.88	0.54
1:B:94:LEU:HD11	1:B:130:VAL:HG21	1.90	0.54
1:B:729:GLY:O	1:B:736:PHE:HB2	2.07	0.54
1:A:749:HIS:O	1:A:752:ARG:N	2.41	0.54
1:B:275:LYS:HG3	1:B:513:TYR:CE2	2.42	0.54
1:A:156:SER:HA	1:A:160:LEU:HD12	1.89	0.54
1:A:563:GLN:HE21	1:A:584:THR:HA	1.72	0.54
1:B:635:THR:CB	1:B:637:PRO:HD2	2.37	0.54
1:A:51:GLU:OE1	1:A:51:GLU:HA	2.08	0.54
1:A:72:GLU:O	1:A:75:LYS:HB3	2.07	0.54
1:A:146:ASN:O	1:A:149:TYR:HB3	2.08	0.54
1:A:674:GLY:HA2	3:A:9002:SD2:OAT	2.07	0.54
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.36	0.54
1:A:440:ASN:ND2	1:A:493:ALA:HB2	2.23	0.54
1:A:563:GLN:O	1:A:566:ILE:HG22	2.08	0.54
1:B:221:PHE:CE2	1:B:225:ILE:HG13	2.42	0.54
1:B:280:HIS:C	1:B:282:SER:N	2.60	0.54
1:A:150:GLU:OE2	1:A:153:LYS:HE2	2.07	0.53
1:A:612:SER:O	1:A:616:LYS:HG3	2.08	0.53
1:A:614:LEU:O	1:A:618:VAL:HG23	2.08	0.53
1:B:410:LYS:O	1:B:414:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LYS:HE3	1:A:532:VAL:O	2.07	0.53
1:B:77:ILE:HG22	1:B:127:PRO:HG2	1.90	0.53
1:A:585:PHE:CZ	1:A:596:VAL:HG13	2.44	0.53
1:A:608:ASN:N	1:A:608:ASN:ND2	2.56	0.53
1:B:467:ILE:O	1:B:468:PHE:C	2.45	0.53
1:A:314:GLU:HA	1:A:317:GLU:CG	2.38	0.53
1:A:636:LEU:C	1:A:638:ASN:H	2.11	0.53
1:A:670:GLY:H	1:A:671:PRO:CD	2.20	0.53
1:A:265:LEU:O	1:A:269:GLU:HB2	2.08	0.53
1:A:314:GLU:HA	1:A:317:GLU:HG2	1.89	0.53
1:B:468:PHE:CE1	1:B:534:ILE:HG13	2.44	0.53
1:B:478:SER:O	1:B:527:LEU:HB2	2.08	0.53
1:A:167:TYR:HD2	1:A:168:GLN:H	1.57	0.53
1:A:204:GLU:O	1:A:207:GLU:HB3	2.09	0.53
1:B:468:PHE:CE1	1:B:534:ILE:HG12	2.44	0.53
1:B:636:LEU:O	1:B:637:PRO:C	2.46	0.53
1:B:737:PHE:CE1	1:B:766:ILE:HG13	2.43	0.53
1:A:190:PHE:CD1	1:A:194:LEU:HB3	2.44	0.53
1:A:210:SER:O	1:A:214:GLN:HG3	2.08	0.53
1:A:677:LEU:HD11	3:A:9002:SD2:CAN	2.39	0.53
1:B:243:TYR:CD1	1:B:244:MET:N	2.77	0.53
1:B:610:ILE:HD12	1:B:610:ILE:N	2.22	0.53
1:A:223:TYR:HB3	1:A:233:LEU:HD12	1.91	0.53
1:A:293:LEU:O	1:A:296:LEU:HB3	2.09	0.53
1:A:567:ASN:C	1:A:569:GLU:N	2.62	0.53
1:B:40:MET:HA	1:B:44:VAL:HG23	1.90	0.53
1:B:720:GLU:OE2	1:B:761:LYS:HE2	2.08	0.53
1:A:443:ILE:HD11	1:A:471:PHE:CD1	2.44	0.53
1:B:640:ALA:HA	1:B:643:TYR:CZ	2.44	0.53
1:B:675:VAL:HG23	3:B:9003:SD2:NBF	2.23	0.53
1:A:146:ASN:O	1:A:147:VAL:C	2.46	0.53
1:A:237:ALA:HB1	1:A:240:ALA:HB3	1.91	0.53
1:A:693:ASP:OD1	1:A:709:THR:HG22	2.09	0.53
1:B:77:ILE:CG2	1:B:127:PRO:HG2	2.39	0.53
1:B:91:HIS:NE2	1:B:93:SER:HB2	2.24	0.53
1:B:243:TYR:HD1	1:B:244:MET:N	2.07	0.53
1:B:448:ALA:HB3	1:B:672:SER:O	2.09	0.53
1:A:233:LEU:HD23	1:A:237:ALA:CB	2.40	0.52
1:A:253:ASN:C	1:A:255:SER:H	2.12	0.52
1:A:82:TYR:HB2	1:A:130:VAL:HG22	1.90	0.52
1:A:681:SER:O	1:A:684:PHE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:MET:SD	1:B:446:LEU:HD13	2.48	0.52
1:B:636:LEU:N	1:B:636:LEU:CD1	2.72	0.52
1:A:429:SER:HB3	1:A:432:TYR:CZ	2.44	0.52
1:A:460:ASN:O	1:A:498:ARG:NH2	2.40	0.52
1:B:463:ILE:HG13	1:B:541:GLU:HB3	1.92	0.52
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.09	0.52
1:A:278:TYR:C	1:A:280:HIS:H	2.13	0.52
1:A:286:SER:C	1:A:288:GLU:H	2.11	0.52
1:A:437:LEU:HD12	1:A:505:LEU:HD21	1.92	0.52
1:B:614:LEU:HD13	1:B:770:ILE:HG23	1.90	0.52
1:A:155:LEU:O	1:A:160:LEU:HG	2.09	0.52
1:B:461:THR:O	1:B:541:GLU:HB2	2.10	0.52
1:B:673:LYS:O	1:B:674:GLY:C	2.46	0.52
1:A:103:LYS:HG3	1:A:113:LEU:CD2	2.40	0.52
1:A:584:THR:HG21	1:A:630:VAL:HG22	1.92	0.52
1:B:46:ILE:HG22	1:B:48:VAL:HG13	1.91	0.52
1:A:314:GLU:O	1:A:318:LEU:HG	2.09	0.52
1:A:701:ASP:O	1:A:703:ASN:N	2.42	0.52
1:B:570:TRP:CZ3	1:B:574:LEU:HD21	2.44	0.52
1:A:196:GLU:O	1:A:197:HIS:C	2.48	0.52
1:A:212:GLU:O	1:A:215:GLU:HB3	2.10	0.52
1:A:253:ASN:C	1:A:255:SER:N	2.62	0.52
1:A:335:LYS:C	1:A:337:PHE:N	2.63	0.52
1:A:335:LYS:O	1:A:337:PHE:N	2.43	0.52
1:A:505:LEU:N	1:A:505:LEU:HD22	2.25	0.52
1:B:324:ILE:HG22	1:B:325:ASP:N	2.24	0.52
1:B:640:ALA:HB2	1:B:643:TYR:CZ	2.45	0.52
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.44	0.52
1:B:319:LEU:CD2	1:B:345:ILE:HD11	2.39	0.52
1:B:416:ILE:O	1:B:418:ASN:N	2.42	0.52
1:B:632:THR:OG1	1:B:633:ASP:N	2.43	0.52
1:B:732:ASN:OD1	1:B:734:ALA:N	2.43	0.52
1:A:55:LYS:HD2	1:A:133:SER:OG	2.10	0.51
1:A:456:ASP:OD1	1:A:464:ASN:HB2	2.10	0.51
1:A:468:PHE:HD1	1:A:543:ILE:HD11	1.75	0.51
1:B:276:GLN:NE2	1:B:431:LEU:HD11	2.25	0.51
1:B:174:LEU:HD22	1:B:216:VAL:HG11	1.92	0.51
1:B:178:LYS:O	1:B:178:LYS:HG3	2.09	0.51
1:B:493:ALA:O	1:B:494:LEU:HD23	2.10	0.51
1:B:640:ALA:HA	1:B:643:TYR:CE1	2.45	0.51
1:A:73:MET:CB	1:A:159:ILE:HD13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:MET:O	1:A:267:ARG:N	2.44	0.51
1:A:437:LEU:HD12	1:A:505:LEU:CD2	2.40	0.51
1:B:66:VAL:HG21	1:B:151:ILE:HD13	1.91	0.51
1:B:121:ALA:HB2	1:B:150:GLU:HG3	1.92	0.51
1:B:278:TYR:CE2	1:B:511:ALA:O	2.61	0.51
1:B:601:LEU:O	1:B:604:ASN:N	2.39	0.51
1:A:509:THR:OG1	1:A:549:VAL:HG11	2.11	0.51
1:B:552:LYS:C	1:B:554:LYS:H	2.14	0.51
1:A:32:GLN:O	1:A:36:LEU:HB2	2.10	0.51
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.91	0.51
1:B:592:ALA:O	1:B:593:SER:C	2.49	0.51
1:B:293:LEU:O	1:B:297:GLN:HG3	2.11	0.51
1:B:762:THR:HG22	1:B:766:ILE:HD13	1.91	0.51
1:A:374:GLU:O	1:A:377:LYS:HB2	2.11	0.51
1:A:442:ASN:HB2	1:A:496:ASN:ND2	2.22	0.51
1:B:426:SER:HA	1:B:509:THR:O	2.10	0.51
1:A:500:LYS:NZ	1:A:544:ARG:NH2	2.58	0.51
1:A:584:THR:HG22	1:A:629:PHE:O	2.11	0.51
1:A:634:ILE:O	1:A:635:THR:C	2.48	0.51
1:B:62:LEU:HD13	1:B:63:LEU:HD23	1.93	0.51
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.43	0.51
1:B:463:ILE:HD11	1:B:541:GLU:C	2.32	0.51
1:B:729:GLY:HA2	1:B:739:GLU:HG3	1.93	0.51
1:A:156:SER:HB3	1:A:217:PHE:HD2	1.75	0.51
1:B:304:LYS:O	1:B:308:ILE:HG13	2.11	0.51
1:B:520:ILE:HG23	1:B:520:ILE:O	2.11	0.51
1:A:83:ILE:HA	1:A:131:ILE:O	2.11	0.51
1:A:296:LEU:HD23	1:A:296:LEU:O	2.11	0.51
1:A:505:LEU:N	1:A:505:LEU:CD2	2.74	0.51
1:B:304:LYS:HD3	1:B:304:LYS:N	2.23	0.50
1:A:294:LYS:O	1:A:297:GLN:N	2.44	0.50
1:A:516:ASN:ND2	1:A:518:LYS:HD2	2.26	0.50
1:B:311:LEU:HD22	1:B:315:GLU:HB3	1.94	0.50
1:B:721:GLU:OE1	1:B:761:LYS:HB2	2.10	0.50
1:B:226:GLU:CD	1:B:229:HIS:HD1	2.14	0.50
1:B:660:VAL:O	1:B:664:ARG:N	2.44	0.50
1:A:522:GLN:HG3	1:A:523:ARG:O	2.10	0.50
1:B:269:GLU:O	1:B:273:LYS:HG2	2.12	0.50
1:A:755:VAL:O	1:A:759:ALA:HB3	2.11	0.50
1:B:192:ASN:C	1:B:194:LEU:H	2.14	0.50
1:B:300:ILE:HB	1:B:386:TYR:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD12	1:A:505:LEU:HG	1.93	0.50
1:B:379:LEU:O	1:B:380:LYS:C	2.49	0.50
1:A:404:ILE:O	1:A:405:ASN:O	2.30	0.50
1:A:718:PHE:CD1	1:A:733:GLU:HB3	2.47	0.50
1:A:737:PHE:HD2	1:A:737:PHE:O	1.95	0.50
1:B:87:ASP:O	1:B:90:LYS:HG2	2.12	0.50
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.46	0.50
1:A:279:GLN:O	1:A:279:GLN:HG3	2.11	0.50
1:B:319:LEU:HD21	1:B:341:LEU:HD22	1.94	0.50
1:B:390:GLN:NE2	1:B:390:GLN:HA	2.27	0.50
1:B:713:LYS:O	1:B:717:ILE:HD11	2.12	0.50
1:A:87:ASP:CG	1:A:89:THR:HG1	2.14	0.49
1:B:729:GLY:CA	1:B:739:GLU:HG3	2.42	0.49
1:A:59:ALA:HB1	1:A:83:ILE:CD1	2.38	0.49
1:A:637:PRO:HB3	1:A:652:GLN:NE2	2.27	0.49
1:B:303:LYS:HD3	1:B:304:LYS:HZ1	1.76	0.49
1:B:610:ILE:HB	1:B:615:ILE:HD11	1.93	0.49
1:A:30:LYS:O	1:A:30:LYS:CG	2.61	0.49
1:A:440:ASN:HD21	1:A:500:LYS:CE	2.12	0.49
1:B:125:TYR:HE2	1:B:162:LYS:HE3	1.77	0.49
1:A:185:GLY:HA3	1:A:236:TYR:O	2.13	0.49
1:A:505:LEU:HD12	1:A:509:THR:HG21	1.93	0.49
1:A:658:LEU:CD2	1:A:659:TYR:N	2.76	0.49
1:A:78:GLY:O	1:A:127:PRO:HD2	2.12	0.49
1:A:86:GLY:O	1:A:132:GLN:NE2	2.45	0.49
1:A:298:ILE:HD12	1:A:299:PRO:O	2.12	0.49
1:B:123:GLU:HG3	1:B:157:ARG:HH11	1.76	0.49
1:B:714:PHE:CE2	1:B:733:GLU:HB2	2.47	0.49
3:B:9003:SD2:OAT	3:B:9003:SD2:CAL	2.54	0.49
1:A:202:SER:HB2	1:A:204:GLU:OE2	2.13	0.49
1:B:83:ILE:HD12	1:B:131:ILE:CG2	2.42	0.49
1:B:681:SER:O	1:B:685:ILE:HG13	2.12	0.49
1:A:152:GLY:O	1:A:153:LYS:C	2.50	0.49
1:A:153:LYS:O	1:A:157:ARG:HB3	2.13	0.49
1:A:252:ILE:CG2	1:A:253:ASN:N	2.76	0.49
1:A:528:GLU:OE1	1:A:550:VAL:HG21	2.13	0.49
1:A:733:GLU:HG2	1:A:734:ALA:H	1.78	0.49
1:B:40:MET:O	1:B:44:VAL:HB	2.13	0.49
1:B:759:ALA:N	1:B:760:PRO:HD3	2.27	0.49
1:A:169:LYS:HE3	1:A:533:GLN:CB	2.43	0.49
1:A:177:ILE:HD12	1:A:238:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PHE:N	1:A:244:MET:HE2	2.28	0.49
1:A:314:GLU:C	1:A:317:GLU:HG2	2.33	0.49
1:A:572:LYS:C	1:A:574:LEU:H	2.16	0.49
1:A:65:LYS:HE2	1:A:227:PRO:HG3	1.95	0.49
1:A:163:ILE:O	1:A:164:ASN:HB2	2.13	0.49
1:A:278:TYR:O	1:A:280:HIS:N	2.46	0.49
1:A:508:ASP:O	1:A:509:THR:C	2.51	0.49
1:B:91:HIS:CG	1:B:93:SER:H	2.31	0.49
1:A:443:ILE:HG13	1:A:499:LEU:HD21	1.95	0.48
1:B:194:LEU:O	1:B:194:LEU:HG	2.12	0.48
1:B:487:ASP:OD1	1:B:518:LYS:HE2	2.13	0.48
1:B:730:ARG:O	1:B:731:THR:O	2.31	0.48
1:A:477:TYR:H	1:A:593:SER:CB	2.12	0.48
1:A:696:ALA:O	1:A:699:LEU:N	2.46	0.48
1:B:40:MET:HA	1:B:43:ILE:HG12	1.95	0.48
1:A:124:GLY:C	1:A:126:GLU:H	2.15	0.48
1:A:209:ASN:O	1:A:212:GLU:HB2	2.14	0.48
1:A:442:ASN:CG	1:A:496:ASN:HB2	2.34	0.48
1:A:589:ASN:HB2	1:A:633:ASP:OD2	2.13	0.48
1:A:713:LYS:O	1:A:717:ILE:HG13	2.13	0.48
1:B:226:GLU:OE1	1:B:229:HIS:ND1	2.36	0.48
1:B:596:VAL:O	1:B:599:ALA:HB3	2.13	0.48
1:B:718:PHE:CG	1:B:733:GLU:HB3	2.49	0.48
1:B:40:MET:C	1:B:42:HIS:H	2.17	0.48
1:B:366:ASN:ND2	1:B:367:PRO:HD2	2.26	0.48
1:B:721:GLU:HA	1:B:724:ASN:OD1	2.12	0.48
1:A:107:ILE:CG2	1:A:108:TYR:N	2.72	0.48
1:A:465:ARG:O	1:A:469:ASN:ND2	2.46	0.48
1:B:102:LYS:O	1:B:113:LEU:HD22	2.13	0.48
1:B:312:SER:O	1:B:313:GLN:C	2.51	0.48
1:B:682:GLU:HA	1:B:685:ILE:HD12	1.95	0.48
1:A:76:ALA:C	1:A:78:GLY:N	2.66	0.48
1:A:442:ASN:CB	1:A:496:ASN:HD22	2.21	0.48
1:B:229:HIS:O	1:B:232:VAL:HG23	2.13	0.48
1:B:447:THR:HG23	1:B:447:THR:O	2.13	0.48
1:B:675:VAL:HG12	1:B:676:GLU:HG2	1.95	0.48
1:A:267:ARG:HE	1:A:491:ARG:HH21	1.60	0.48
1:A:489:ASN:O	1:A:490:GLU:C	2.51	0.48
1:B:314:GLU:HG3	1:B:314:GLU:O	2.13	0.48
1:B:498:ARG:NH1	1:B:540:LYS:HE3	2.28	0.48
1:A:187:ASP:HA	1:A:195:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:O	1:A:317:GLU:HG2	2.14	0.48
1:A:636:LEU:O	1:A:638:ASN:N	2.47	0.48
1:B:322:ILE:HG13	1:B:372:GLU:OE2	2.14	0.48
1:B:369:SER:C	1:B:371:LYS:H	2.17	0.48
1:B:635:THR:HG22	1:B:654:HIS:CE1	2.48	0.48
1:A:733:GLU:H	1:A:733:GLU:CD	2.17	0.48
1:B:476:LYS:O	1:B:529:ILE:HB	2.14	0.48
1:B:715:ILE:O	1:B:718:PHE:HB3	2.13	0.48
1:A:553:SER:O	1:A:554:LYS:C	2.51	0.48
1:A:741:PHE:O	1:A:744:MET:N	2.47	0.48
1:B:65:LYS:HB3	1:B:225:ILE:HG22	1.95	0.48
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.13	0.48
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.44	0.48
1:B:529:ILE:N	1:B:529:ILE:HD12	2.29	0.48
1:B:669:HIS:CE1	1:B:671:PRO:HD2	2.49	0.48
1:A:107:ILE:HG22	1:A:146:ASN:OD1	2.14	0.47
1:A:199:THR:OG1	1:A:200:ASP:N	2.47	0.47
1:A:688:PHE:O	1:A:691:ALA:HB3	2.13	0.47
1:B:243:TYR:C	1:B:243:TYR:CD1	2.86	0.47
1:B:749:HIS:O	1:B:752:ARG:N	2.44	0.47
1:A:51:GLU:O	1:A:53:ALA:N	2.47	0.47
1:A:87:ASP:OD2	1:A:89:THR:N	2.47	0.47
1:A:256:LEU:HD13	1:A:256:LEU:C	2.34	0.47
1:A:294:LYS:O	1:A:295:LYS:C	2.52	0.47
1:A:732:ASN:OD1	1:A:732:ASN:C	2.52	0.47
1:A:770:ILE:O	1:A:774:ILE:HG13	2.14	0.47
1:B:43:ILE:HG13	1:B:44:VAL:N	2.28	0.47
1:B:636:LEU:CD1	1:B:636:LEU:H	2.27	0.47
1:B:679:ASN:O	1:B:682:GLU:N	2.46	0.47
1:B:275:LYS:HG3	1:B:513:TYR:HE2	1.79	0.47
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.14	0.47
1:B:498:ARG:HH12	1:B:540:LYS:HG2	1.79	0.47
1:A:286:SER:C	1:A:288:GLU:N	2.68	0.47
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.44	0.47
1:A:657:GLY:HA2	1:A:667:LEU:O	2.14	0.47
1:B:202:SER:C	1:B:204:GLU:N	2.66	0.47
1:B:749:HIS:O	1:B:750:ALA:C	2.52	0.47
1:A:118:TYR:OH	1:A:143:LYS:HA	2.14	0.47
1:B:530:LYS:O	1:B:531:ASP:HB2	2.14	0.47
1:B:587:VAL:O	1:B:588:HIS:CG	2.67	0.47
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:NH1	1:A:404:ILE:CD1	2.78	0.47
1:B:91:HIS:NE2	1:B:93:SER:CB	2.76	0.47
1:B:674:GLY:O	1:B:677:LEU:HB2	2.14	0.47
1:A:104:ILE:HG13	1:A:120:TYR:CE1	2.50	0.47
1:A:258:GLU:CG	1:A:502:ARG:HH12	2.25	0.47
1:A:327:SER:HB2	1:A:329:PHE:CE2	2.49	0.47
1:A:401:SER:O	1:A:403:SER:N	2.37	0.47
1:A:656:LYS:O	1:A:668:LEU:HD12	2.14	0.47
1:A:718:PHE:O	1:A:722:GLY:HA3	2.15	0.47
1:B:107:ILE:HG12	1:B:149:TYR:CD1	2.49	0.47
1:B:338:LEU:HD21	1:B:379:LEU:HB3	1.96	0.47
1:B:654:HIS:O	3:B:9003:SD2:HBE3	2.15	0.47
1:A:191:THR:HG23	1:A:194:LEU:H	1.80	0.47
1:A:550:VAL:HG12	1:A:551:PRO:CD	2.43	0.47
1:B:123:GLU:CG	1:B:124:GLY:H	2.28	0.47
1:A:476:LYS:N	1:A:593:SER:OG	2.34	0.47
1:A:693:ASP:OD2	1:A:693:ASP:O	2.33	0.47
1:A:693:ASP:CG	1:A:708:VAL:HG12	2.36	0.47
1:A:718:PHE:HA	1:A:722:GLY:HA3	1.97	0.47
1:A:725:LEU:HD12	1:A:736:PHE:CE1	2.50	0.47
1:B:84:VAL:HG22	1:B:85:ASP:N	2.30	0.47
1:B:129:LEU:HD23	1:B:129:LEU:C	2.35	0.47
1:B:511:ALA:CB	1:B:521:LEU:HA	2.45	0.47
1:B:564:LEU:O	1:B:568:GLN:HB2	2.15	0.47
1:A:118:TYR:CD1	1:A:118:TYR:N	2.83	0.47
1:A:338:LEU:CD2	1:A:383:ILE:HG21	2.45	0.47
1:A:479:ILE:HG22	1:A:480:SER:N	2.30	0.47
1:A:495:ASP:C	1:A:497:GLU:N	2.68	0.47
1:B:660:VAL:HG13	1:B:662:GLU:OE2	2.14	0.47
1:A:81:ILE:HG12	1:A:129:LEU:HD23	1.98	0.46
1:A:87:ASP:OD2	1:A:87:ASP:C	2.52	0.46
1:A:191:THR:HG21	1:A:212:GLU:OE2	2.15	0.46
1:B:280:HIS:O	1:B:282:SER:N	2.48	0.46
1:B:614:LEU:O	1:B:618:VAL:HG23	2.14	0.46
1:A:639:ILE:HG23	1:A:641:GLU:OE1	2.15	0.46
1:A:696:ALA:O	1:A:697:GLY:C	2.53	0.46
1:B:189:LEU:HD22	1:B:220:ALA:HB2	1.97	0.46
1:B:276:GLN:O	1:B:277:HIS:C	2.54	0.46
1:A:498:ARG:CD	1:A:542:TYR:CD2	2.97	0.46
1:A:639:ILE:HG21	1:A:667:LEU:HD21	1.96	0.46
1:A:683:GLY:O	1:A:687:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLN:C	1:B:34:GLU:H	2.18	0.46
1:B:472:LYS:HG3	1:B:473:LYS:N	2.29	0.46
1:B:526:GLY:HA3	1:B:550:VAL:O	2.16	0.46
1:A:191:THR:C	1:A:193:GLN:H	2.19	0.46
1:A:437:LEU:HD12	1:A:505:LEU:CG	2.46	0.46
1:A:586:ASN:HB3	1:A:632:THR:OG1	2.14	0.46
1:A:636:LEU:C	1:A:638:ASN:N	2.67	0.46
1:A:718:PHE:CE1	1:A:733:GLU:N	2.84	0.46
1:B:261:ASP:OD1	1:B:490:GLU:HB3	2.15	0.46
1:B:455:VAL:HG22	1:B:498:ARG:HE	1.79	0.46
1:A:264:MET:O	1:A:265:LEU:C	2.54	0.46
1:A:272:GLU:HG3	1:B:125:TYR:CE1	2.51	0.46
1:A:446:LEU:HG	1:A:591:TYR:HB2	1.98	0.46
1:B:77:ILE:HG22	1:B:77:ILE:O	2.16	0.46
1:B:331:SER:HB3	1:B:334:GLU:HB2	1.97	0.46
1:B:366:ASN:CG	1:B:367:PRO:HD3	2.34	0.46
1:B:488:ILE:HG22	1:B:489:ASN:CG	2.36	0.46
1:B:640:ALA:C	1:B:642:GLN:N	2.69	0.46
1:A:316:LYS:O	1:A:319:LEU:HB3	2.15	0.46
1:A:410:LYS:NZ	1:A:414:ARG:HH21	2.14	0.46
1:A:439:GLU:OE1	1:A:590:ARG:NH2	2.49	0.46
1:A:498:ARG:HG2	1:A:498:ARG:HH11	1.81	0.46
1:A:674:GLY:O	1:A:675:VAL:C	2.53	0.46
1:B:331:SER:HB3	1:B:334:GLU:CD	2.36	0.46
1:B:769:GLN:O	1:B:772:PHE:HB3	2.16	0.46
1:A:54:VAL:O	1:A:57:GLU:HB3	2.16	0.46
1:A:57:GLU:O	1:A:61:LYS:N	2.36	0.46
1:A:311:LEU:O	1:A:312:SER:HB3	2.15	0.46
1:B:171:LEU:O	1:B:175:ASN:HB2	2.15	0.46
1:B:238:PRO:O	1:B:241:PHE:HB3	2.15	0.46
1:B:247:PHE:CE2	1:B:252:ILE:HD13	2.51	0.46
1:B:468:PHE:CG	1:B:534:ILE:HD11	2.51	0.46
1:A:529:ILE:HD13	1:A:529:ILE:N	2.31	0.46
1:B:294:LYS:HG3	1:B:295:LYS:N	2.31	0.46
1:B:735:GLU:O	1:B:736:PHE:C	2.52	0.46
1:A:62:LEU:HD21	1:A:147:VAL:HG11	1.97	0.46
1:A:592:ALA:HA	1:A:595:ILE:HG12	1.97	0.46
1:A:167:TYR:OH	1:A:536:LYS:HB2	2.15	0.46
1:B:376:LEU:HD23	1:B:379:LEU:HD12	1.98	0.46
1:B:636:LEU:N	1:B:637:PRO:CD	2.79	0.46
1:A:46:ILE:O	1:A:47:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:O	1:A:78:GLY:N	2.49	0.45
1:A:205:PHE:CE2	1:A:209:ASN:ND2	2.82	0.45
1:A:753:LEU:O	1:A:756:GLN:N	2.48	0.45
1:B:557:THR:HA	1:B:560:GLN:HG2	1.97	0.45
1:A:481:SER:HA	1:A:524:ASN:HD22	1.80	0.45
1:A:615:ILE:HG22	1:A:616:LYS:N	2.31	0.45
1:B:643:TYR:HB3	1:B:646:GLN:OE1	2.16	0.45
1:B:670:GLY:H	1:B:671:PRO:CD	2.28	0.45
1:A:126:GLU:O	1:A:126:GLU:HG3	2.16	0.45
1:A:314:GLU:CA	1:A:317:GLU:HG2	2.46	0.45
1:A:427:ILE:CG2	1:A:428:GLY:H	2.30	0.45
1:A:615:ILE:O	1:A:619:THR:HG23	2.15	0.45
1:A:695:TYR:O	1:A:698:TYR:HB3	2.17	0.45
1:A:191:THR:OG1	1:A:192:ASN:N	2.50	0.45
1:A:299:PRO:O	1:A:300:ILE:HG23	2.16	0.45
1:B:49:LYS:HB2	1:B:50:GLY:H	1.58	0.45
1:B:239:GLU:O	1:B:242:ASN:N	2.49	0.45
1:B:369:SER:O	1:B:371:LYS:N	2.49	0.45
1:A:88:ILE:HD13	1:A:118:TYR:C	2.36	0.45
1:A:122:LYS:CB	1:A:128:VAL:HB	2.47	0.45
1:A:220:ALA:C	1:A:244:MET:HE2	2.37	0.45
1:A:264:MET:O	1:A:266:SER:N	2.49	0.45
1:A:584:THR:HG23	1:A:630:VAL:HA	1.98	0.45
1:A:682:GLU:O	1:A:685:ILE:N	2.44	0.45
1:B:467:ILE:HD12	1:B:467:ILE:N	2.32	0.45
1:B:487:ASP:OD2	1:B:487:ASP:N	2.49	0.45
1:B:731:THR:HG22	1:B:732:ASN:H	1.81	0.45
1:A:429:SER:HB3	1:A:432:TYR:CE1	2.52	0.45
1:B:51:GLU:O	1:B:53:ALA:N	2.50	0.45
1:B:74:TYR:CZ	1:B:79:GLY:HA3	2.52	0.45
1:B:563:GLN:NE2	1:B:584:THR:HA	2.32	0.45
1:B:717:ILE:N	1:B:717:ILE:HD13	2.31	0.45
1:A:191:THR:HG22	1:A:194:LEU:CG	2.47	0.45
1:A:264:MET:HG2	1:A:265:LEU:N	2.31	0.45
1:B:89:THR:HG21	1:B:97:LEU:HD12	1.98	0.45
1:B:211:ASN:O	1:B:214:GLN:N	2.49	0.45
1:B:264:MET:O	1:B:267:ARG:N	2.48	0.45
1:B:427:ILE:HG23	1:B:428:GLY:H	1.80	0.45
1:B:477:TYR:N	1:B:593:SER:HB2	2.30	0.45
1:B:505:LEU:HD11	1:B:521:LEU:HD21	1.98	0.45
1:A:73:MET:O	1:A:76:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ILE:HG13	1:A:600:TYR:CE2	2.52	0.45
1:A:739:GLU:O	1:A:743:LEU:CD1	2.65	0.45
1:B:303:LYS:HD3	1:B:304:LYS:NZ	2.32	0.45
1:B:467:ILE:HD12	1:B:467:ILE:H	1.82	0.45
1:A:61:LYS:HA	1:A:61:LYS:CE	2.45	0.45
1:A:426:SER:HB3	1:A:508:ASP:O	2.17	0.45
1:A:611:GLN:NE2	1:A:774:ILE:HD11	2.29	0.45
1:A:707:LEU:HD23	1:A:707:LEU:H	1.81	0.45
1:B:587:VAL:HG11	1:B:592:ALA:HA	1.99	0.45
1:A:197:HIS:HA	1:A:198:PRO:HD3	1.85	0.44
1:A:366:ASN:HB2	1:A:367:PRO:HD3	1.99	0.44
1:A:744:MET:SD	1:A:766:ILE:HG21	2.57	0.44
1:A:766:ILE:HD12	1:A:766:ILE:N	2.32	0.44
1:B:762:THR:C	1:B:764:GLN:N	2.70	0.44
1:A:169:LYS:HE3	1:A:533:GLN:HB2	2.00	0.44
1:A:187:ASP:HA	1:A:195:LYS:CE	2.47	0.44
1:A:188:LEU:HD12	1:A:188:LEU:O	2.18	0.44
1:A:462:LYS:HA	1:A:541:GLU:OE2	2.17	0.44
1:B:48:VAL:HB	1:B:49:LYS:H	1.51	0.44
1:A:311:LEU:O	1:A:315:GLU:HB2	2.17	0.44
1:B:131:ILE:HD11	1:B:147:VAL:HG11	1.99	0.44
1:B:594:ASN:O	1:B:595:ILE:C	2.55	0.44
1:B:679:ASN:O	1:B:680:ASP:C	2.56	0.44
1:B:766:ILE:HG22	1:B:767:ASN:N	2.31	0.44
1:A:185:GLY:CA	1:A:236:TYR:O	2.66	0.44
1:A:255:SER:O	1:A:256:LEU:C	2.55	0.44
1:A:427:ILE:O	1:A:428:GLY:C	2.54	0.44
1:A:588:HIS:C	1:A:589:ASN:HD22	2.20	0.44
1:B:155:LEU:HD12	1:B:159:ILE:CG2	2.47	0.44
1:B:176:THR:O	1:B:180:ALA:N	2.46	0.44
1:B:479:ILE:O	1:B:589:ASN:C	2.56	0.44
1:B:591:TYR:O	1:B:595:ILE:HG12	2.17	0.44
1:B:658:LEU:HD23	1:B:659:TYR:N	2.32	0.44
1:B:721:GLU:OE2	1:B:760:PRO:N	2.51	0.44
1:A:639:ILE:HG21	1:A:667:LEU:HD22	2.00	0.44
1:A:711:SER:OG	1:A:714:PHE:HB2	2.17	0.44
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.99	0.44
1:B:640:ALA:CA	1:B:643:TYR:CZ	3.01	0.44
1:A:371:LYS:HD2	1:A:371:LYS:HA	1.81	0.44
1:A:391:ARG:NH1	1:A:404:ILE:HD13	2.33	0.44
1:A:566:ILE:HG12	1:A:566:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:PRO:O	1:A:664:ARG:HG3	2.17	0.44
1:B:122:LYS:HB3	1:B:128:VAL:HG23	1.99	0.44
1:B:640:ALA:HB2	1:B:643:TYR:OH	2.17	0.44
1:B:693:ASP:HB2	1:B:737:PHE:CE2	2.52	0.44
1:A:31:THR:HG22	1:A:32:GLN:N	2.32	0.44
1:A:523:ARG:O	1:A:524:ASN:HB2	2.17	0.44
1:A:765:PHE:O	1:A:768:ASP:HB3	2.17	0.44
1:B:466:GLY:O	1:B:467:ILE:C	2.56	0.44
1:B:758:ASN:C	1:B:760:PRO:HD3	2.37	0.44
1:B:113:LEU:HB2	1:B:116:GLU:OE1	2.18	0.44
1:B:511:ALA:HB2	1:B:521:LEU:HA	2.00	0.44
1:A:378:LYS:HG2	1:A:650:TYR:CD2	2.53	0.44
1:A:488:ILE:HG13	1:A:517:GLY:O	2.18	0.44
1:A:506:SER:O	1:A:507:PRO:C	2.56	0.44
1:A:600:TYR:O	1:A:604:ASN:HB2	2.17	0.44
1:B:222:ALA:O	1:B:223:TYR:C	2.56	0.44
1:B:416:ILE:C	1:B:418:ASN:N	2.71	0.44
1:B:505:LEU:HD23	1:B:549:VAL:HG21	1.99	0.44
1:B:670:GLY:N	1:B:671:PRO:CD	2.81	0.44
1:B:765:PHE:O	1:B:768:ASP:HB3	2.18	0.44
1:A:241:PHE:C	1:A:241:PHE:HD1	2.20	0.43
1:A:440:ASN:CG	1:A:493:ALA:HB2	2.38	0.43
1:A:522:GLN:HG2	1:A:525:ILE:HD11	1.99	0.43
1:A:660:VAL:HA	1:A:661:PRO:HD3	1.91	0.43
1:B:503:ILE:N	1:B:503:ILE:CD1	2.78	0.43
1:A:335:LYS:CG	1:A:336:GLU:N	2.81	0.43
1:B:89:THR:O	1:B:89:THR:HG22	2.18	0.43
1:B:193:GLN:HE21	1:B:193:GLN:HB3	1.61	0.43
1:B:490:GLU:HG3	1:B:491:ARG:N	2.33	0.43
1:B:766:ILE:C	1:B:768:ASP:N	2.71	0.43
1:A:84:VAL:O	1:A:133:SER:N	2.51	0.43
1:A:500:LYS:HB3	1:A:544:ARG:HH21	1.83	0.43
1:A:614:LEU:HD22	1:A:770:ILE:HD12	2.00	0.43
1:B:412:TYR:O	1:B:416:ILE:HG12	2.18	0.43
1:B:640:ALA:C	1:B:642:GLN:H	2.20	0.43
1:A:154:ILE:HA	1:A:158:ASP:OD1	2.19	0.43
1:A:345:ILE:O	1:A:345:ILE:HG22	2.18	0.43
1:B:84:VAL:C	1:B:133:SER:HB3	2.37	0.43
1:B:468:PHE:O	1:B:471:PHE:HB3	2.18	0.43
1:A:145:LEU:HD22	1:A:229:HIS:NE2	2.33	0.43
1:A:741:PHE:O	1:A:742:ARG:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASP:O	1:B:419:ILE:HG13	2.19	0.43
1:A:435:ILE:HG22	1:A:437:LEU:HG	2.01	0.43
1:A:479:ILE:CG2	1:A:480:SER:N	2.82	0.43
1:A:634:ILE:HG13	1:A:635:THR:O	2.18	0.43
1:A:640:ALA:HA	1:A:643:TYR:CZ	2.53	0.43
1:A:714:PHE:O	1:A:717:ILE:N	2.39	0.43
1:B:83:ILE:HG23	1:B:131:ILE:CG2	2.47	0.43
1:B:155:LEU:HD12	1:B:159:ILE:HB	2.01	0.43
1:B:297:GLN:OE1	1:B:514:LEU:HD13	2.19	0.43
1:B:309:HIS:O	1:B:310:SER:HB3	2.18	0.43
1:A:56:LYS:HG3	1:A:56:LYS:O	2.18	0.43
1:A:79:GLY:HA3	1:A:127:PRO:HB2	1.99	0.43
1:A:534:ILE:HG22	1:A:535:ILE:N	2.33	0.43
1:B:79:GLY:HA2	1:B:127:PRO:HB2	2.00	0.43
1:B:239:GLU:O	1:B:240:ALA:C	2.56	0.43
1:B:379:LEU:O	1:B:382:ASP:N	2.51	0.43
1:B:388:ILE:HG23	1:B:416:ILE:HD11	2.00	0.43
1:B:476:LYS:N	1:B:593:SER:OG	2.42	0.43
1:B:610:ILE:HG21	1:B:614:LEU:HD23	1.98	0.43
1:B:679:ASN:C	1:B:681:SER:N	2.72	0.43
1:B:690:HIS:CE1	1:B:735:GLU:OE1	2.72	0.43
1:A:140:ASN:HD21	1:A:143:LYS:NZ	2.16	0.43
1:A:155:LEU:HG	1:A:160:LEU:HD11	2.00	0.43
1:A:234:GLN:HG3	1:A:241:PHE:CD2	2.53	0.43
1:A:429:SER:OG	1:A:430:THR:N	2.52	0.43
1:A:525:ILE:CG2	1:A:526:GLY:N	2.82	0.43
1:B:125:TYR:CE2	1:B:162:LYS:HE3	2.53	0.43
1:B:257:GLU:O	1:B:258:GLU:C	2.54	0.43
1:A:107:ILE:C	1:A:107:ILE:CD1	2.87	0.43
1:A:640:ALA:HA	1:A:643:TYR:CE2	2.54	0.43
1:B:639:ILE:O	1:B:642:GLN:N	2.44	0.43
1:B:766:ILE:O	1:B:768:ASP:N	2.52	0.43
1:A:621:TYR:CE1	1:A:664:ARG:CZ	3.02	0.42
1:B:202:SER:O	1:B:205:PHE:N	2.51	0.42
1:A:480:SER:HB3	1:A:525:ILE:HB	2.00	0.42
1:B:65:LYS:HD2	1:B:65:LYS:HA	1.81	0.42
1:B:117:HIS:CG	1:B:118:TYR:N	2.87	0.42
1:A:29:ASN:C	1:A:31:THR:H	2.21	0.42
1:A:32:GLN:O	1:A:36:LEU:CB	2.68	0.42
1:A:611:GLN:HE22	1:A:770:ILE:CG2	2.32	0.42
1:B:496:ASN:HD22	1:B:496:ASN:C	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:PHE:HZ	1:B:731:THR:O	2.02	0.42
1:A:206:LEU:CD1	1:A:213:VAL:HG11	2.49	0.42
1:A:221:PHE:CE1	1:A:225:ILE:HD11	2.54	0.42
1:A:415:ASP:O	1:A:419:ILE:HG13	2.19	0.42
1:A:555:ILE:N	1:A:555:ILE:HD12	2.34	0.42
1:B:610:ILE:H	1:B:610:ILE:CD1	2.27	0.42
1:B:713:LYS:HD2	1:B:765:PHE:CE1	2.53	0.42
1:B:737:PHE:O	1:B:740:ALA:HB3	2.19	0.42
1:A:467:ILE:H	1:A:467:ILE:CD1	2.33	0.42
1:B:264:MET:C	1:B:266:SER:N	2.73	0.42
1:B:388:ILE:O	1:B:391:ARG:N	2.47	0.42
1:B:436:TYR:CE2	1:B:504:GLN:HB2	2.54	0.42
1:A:77:ILE:CG2	1:A:162:LYS:HD2	2.50	0.42
1:A:190:PHE:HD1	1:A:194:LEU:HB3	1.84	0.42
1:A:311:LEU:O	1:A:312:SER:CB	2.67	0.42
1:A:570:TRP:HH2	1:A:607:LYS:HB2	1.85	0.42
1:A:707:LEU:HD23	1:A:707:LEU:N	2.34	0.42
1:B:60:GLU:O	1:B:62:LEU:N	2.52	0.42
1:B:237:ALA:N	1:B:238:PRO:HD3	2.35	0.42
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.49	0.42
1:A:645:HIS:NE2	1:A:663:SER:HB3	2.34	0.42
1:A:686:HIS:CD2	1:A:686:HIS:C	2.93	0.42
1:B:56:LYS:C	1:B:58:ALA:N	2.73	0.42
1:B:70:VAL:HG22	1:B:252:ILE:HD11	2.02	0.42
1:B:437:LEU:HD11	1:B:519:LEU:HD12	2.02	0.42
1:B:654:HIS:O	3:B:9003:SD2:CBE	2.68	0.42
1:A:159:ILE:HG23	1:A:259:LEU:HD11	2.01	0.42
1:A:366:ASN:H	1:A:367:PRO:CD	2.32	0.42
1:A:469:ASN:ND2	1:A:469:ASN:H	2.15	0.42
1:A:725:LEU:HB2	1:A:736:PHE:HE1	1.83	0.42
1:B:30:LYS:HG3	1:B:30:LYS:O	2.20	0.42
1:B:60:GLU:C	1:B:62:LEU:N	2.72	0.42
1:B:416:ILE:HG22	1:B:420:ASP:OD1	2.20	0.42
1:A:70:VAL:HG12	1:A:252:ILE:HD11	2.01	0.42
1:A:403:SER:HB2	1:A:638:ASN:OD1	2.20	0.42
1:A:693:ASP:OD2	1:A:693:ASP:C	2.58	0.42
1:B:427:ILE:O	1:B:432:TYR:OH	2.35	0.42
1:B:657:GLY:HA2	1:B:667:LEU:O	2.20	0.42
1:A:563:GLN:HE21	1:A:585:PHE:H	1.68	0.42
1:B:190:PHE:CB	1:B:194:LEU:HD23	2.50	0.42
1:B:313:GLN:C	1:B:315:GLU:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LYS:O	1:B:579:TYR:HB2	2.20	0.42
1:B:659:TYR:CE2	1:B:661:PRO:HG3	2.55	0.42
1:B:77:ILE:CG2	1:B:77:ILE:O	2.68	0.41
1:B:303:LYS:CD	1:B:304:LYS:HZ1	2.33	0.41
1:B:498:ARG:HA	1:B:498:ARG:HD2	1.92	0.41
1:B:732:ASN:OD1	1:B:734:ALA:HB3	2.20	0.41
1:A:96:ALA:O	1:A:97:LEU:C	2.59	0.41
1:A:125:TYR:HA	1:B:268:TYR:HE2	1.86	0.41
1:A:560:GLN:O	1:A:561:GLU:C	2.59	0.41
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.55	0.41
1:B:264:MET:O	1:B:266:SER:N	2.53	0.41
1:B:324:ILE:O	1:B:325:ASP:C	2.59	0.41
1:A:567:ASN:O	1:A:569:GLU:N	2.49	0.41
1:B:45:LYS:HD2	1:B:82:TYR:HE2	1.80	0.41
1:B:206:LEU:HD23	1:B:213:VAL:HG21	2.03	0.41
1:B:529:ILE:N	1:B:529:ILE:CD1	2.83	0.41
1:B:619:THR:O	1:B:619:THR:HG22	2.19	0.41
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.19	0.41
1:A:369:SER:OG	1:A:372:GLU:CB	2.67	0.41
1:A:394:ASP:HB3	1:A:635:THR:OG1	2.20	0.41
1:A:618:VAL:O	1:A:621:TYR:HB3	2.20	0.41
1:A:655:SER:HA	3:A:9002:SD2:CBE	2.51	0.41
1:B:388:ILE:HG23	1:B:416:ILE:CD1	2.50	0.41
1:A:118:TYR:CE2	1:A:143:LYS:HB3	2.56	0.41
1:A:178:LYS:HG3	1:A:179:ASN:ND2	2.34	0.41
1:A:733:GLU:HG2	1:A:734:ALA:N	2.35	0.41
1:B:420:ASP:CG	1:B:523:ARG:HH11	2.24	0.41
1:A:114:LEU:C	1:A:116:GLU:H	2.24	0.41
1:A:175:ASN:O	1:A:178:LYS:HG2	2.21	0.41
1:A:272:GLU:HA	1:A:275:LYS:HB3	2.01	0.41
1:A:608:ASN:C	1:A:609:ASN:ND2	2.64	0.41
1:B:114:LEU:HD22	1:B:120:TYR:HB2	2.01	0.41
1:B:174:LEU:CD2	1:B:216:VAL:HG11	2.51	0.41
1:B:467:ILE:H	1:B:467:ILE:CD1	2.33	0.41
1:B:610:ILE:HG23	1:B:614:LEU:HD23	1.99	0.41
1:A:247:PHE:O	1:A:247:PHE:CG	2.73	0.41
1:B:74:TYR:CE1	1:B:79:GLY:HA3	2.55	0.41
1:B:401:SER:CB	1:B:638:ASN:ND2	2.75	0.41
1:B:468:PHE:CD2	1:B:534:ILE:HD11	2.56	0.41
1:A:121:ALA:HA	1:A:129:LEU:HA	2.02	0.41
1:A:235:LEU:HD23	1:A:236:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLU:HA	1:A:302:PRO:HD3	1.84	0.41
1:A:311:LEU:O	1:A:315:GLU:OE1	2.39	0.41
1:A:319:LEU:HD13	1:A:319:LEU:C	2.41	0.41
1:A:563:GLN:NE2	1:A:585:PHE:H	2.17	0.41
1:A:721:GLU:OE1	1:A:759:ALA:HA	2.20	0.41
1:B:257:GLU:HA	1:B:260:LYS:HD3	2.03	0.41
1:B:294:LYS:C	1:B:296:LEU:H	2.22	0.41
1:B:473:LYS:O	1:B:474:ASN:HB2	2.20	0.41
1:B:540:LYS:HD3	1:B:542:TYR:CZ	2.55	0.41
1:B:743:LEU:O	1:B:744:MET:C	2.59	0.41
1:B:755:VAL:HG12	1:B:756:GLN:N	2.34	0.41
1:A:118:TYR:HE2	1:A:143:LYS:HB3	1.86	0.41
1:A:151:ILE:O	1:A:152:GLY:C	2.57	0.41
1:A:169:LYS:HE3	1:A:533:GLN:HB3	2.03	0.41
1:A:241:PHE:HD1	1:A:242:ASN:N	2.18	0.41
1:A:391:ARG:CZ	1:A:395:THR:HG21	2.51	0.41
1:A:427:ILE:HD12	1:A:427:ILE:HA	1.81	0.41
1:A:430:THR:O	1:A:431:LEU:HD23	2.21	0.41
1:A:677:LEU:O	1:A:678:ARG:C	2.59	0.41
1:A:728:TYR:O	1:A:729:GLY:C	2.59	0.41
1:B:27:GLU:O	1:B:27:GLU:CG	2.63	0.41
1:B:143:LYS:O	1:B:147:VAL:HG23	2.21	0.41
1:B:186:GLN:NE2	1:B:195:LYS:HB2	2.25	0.41
1:B:490:GLU:HG2	1:B:537:GLN:HE22	1.86	0.41
1:A:154:ILE:HG22	1:A:155:LEU:N	2.35	0.41
1:A:522:GLN:HG3	1:A:523:ARG:N	2.36	0.41
1:B:235:LEU:HD13	1:B:236:TYR:CD1	2.56	0.41
1:B:341:LEU:O	1:B:341:LEU:HD23	2.21	0.41
1:B:673:LYS:O	1:B:673:LYS:CG	2.68	0.41
1:A:223:TYR:HB3	1:A:233:LEU:CD1	2.50	0.40
1:B:113:LEU:H	1:B:116:GLU:CD	2.25	0.40
1:B:408:VAL:O	1:B:411:GLN:HB3	2.21	0.40
1:A:73:MET:SD	1:A:159:ILE:HG21	2.61	0.40
1:A:511:ALA:HB2	1:A:521:LEU:HD23	2.03	0.40
1:A:634:ILE:HD11	1:A:639:ILE:HD12	2.02	0.40
1:A:681:SER:O	1:A:684:PHE:HB3	2.21	0.40
1:B:106:ASP:OD2	1:B:110:LYS:HB2	2.21	0.40
1:B:343:ILE:HG23	1:B:346:ARG:HD2	2.01	0.40
1:A:467:ILE:N	1:A:467:ILE:HD12	2.36	0.40
1:A:478:SER:OG	1:A:590:ARG:HA	2.20	0.40
1:B:89:THR:HG21	1:B:97:LEU:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLN:HB2	1:B:241:PHE:CE2	2.57	0.40
1:A:640:ALA:O	1:A:644:THR:HG23	2.22	0.40
1:A:749:HIS:O	1:A:750:ALA:C	2.60	0.40
1:B:177:ILE:CG2	1:B:186:GLN:HA	2.51	0.40
1:B:226:GLU:HA	1:B:227:PRO:HD3	1.94	0.40
1:B:256:LEU:O	1:B:257:GLU:C	2.59	0.40
1:B:303:LYS:NZ	1:B:304:LYS:HZ1	2.18	0.40
1:A:266:SER:O	1:A:269:GLU:HB3	2.22	0.40
1:A:278:TYR:C	1:A:280:HIS:N	2.75	0.40
1:A:721:GLU:HA	1:A:724:ASN:OD1	2.22	0.40
1:B:202:SER:O	1:B:203:VAL:C	2.60	0.40
1:B:202:SER:C	1:B:204:GLU:H	2.25	0.40
1:B:322:ILE:O	1:B:342:GLN:NE2	2.53	0.40
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.81	0.40
1:B:510:ARG:HB2	1:B:522:GLN:OE1	2.22	0.40
1:B:511:ALA:CB	1:B:521:LEU:HD23	2.51	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	728/776 (94%)	529 (73%)	144 (20%)	55 (8%)	1 11
1	B	730/776 (94%)	536 (73%)	143 (20%)	51 (7%)	1 14
All	All	1458/1552 (94%)	1065 (73%)	287 (20%)	106 (7%)	1 13

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	92	ILE

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Mol	Chain	Res	Type
1	A	227	PRO
1	A	238	PRO
1	A	405	ASN
1	A	457	SER
1	A	473	LYS
1	A	539	GLU
1	A	675	VAL
1	A	678	ARG
1	A	702	LYS
1	A	720	GLU
1	B	33	GLU
1	B	95	GLU
1	B	211	ASN
1	B	310	SER
1	B	325	ASP
1	B	366	ASN
1	B	495	ASP
1	B	553	SER
1	B	731	THR
1	A	181	SER
1	A	279	GLN
1	A	336	GLU
1	A	369	SER
1	A	428	GLY
1	A	573	ALA
1	A	590	ARG
1	A	615	ILE
1	A	647	ASP
1	A	676	GLU
1	B	35	HIS
1	B	96	ALA
1	B	157	ARG
1	B	168	GLN
1	B	203	VAL
1	B	210	SER
1	B	242	ASN
1	B	250	GLN
1	B	324	ILE
1	B	326	SER
1	B	367	PRO
1	B	370	GLU
1	B	417	GLN

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Mol	Chain	Res	Type
1	B	515	GLU
1	B	592	ALA
1	B	593	SER
1	A	30	LYS
1	A	125	TYR
1	A	254	LEU
1	A	265	LEU
1	A	312	SER
1	A	460	ASN
1	A	509	THR
1	A	568	GLN
1	A	593	SER
1	A	741	PHE
1	A	760	PRO
1	B	48	VAL
1	B	52	GLU
1	B	123	GLU
1	B	187	ASP
1	B	531	ASP
1	B	767	ASN
1	A	114	LEU
1	A	198	PRO
1	A	264	MET
1	A	299	PRO
1	A	300	ILE
1	A	329	PHE
1	A	492	PRO
1	A	682	GLU
1	B	53	ALA
1	B	180	ALA
1	B	200	ASP
1	B	468	PHE
1	B	474	ASN
1	B	666	ILE
1	B	732	ASN
1	A	77	ILE
1	A	164	ASN
1	A	402	PRO
1	A	731	THR
1	A	742	ARG
1	B	142	GLU
1	B	169	LYS

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Mol	Chain	Res	Type
1	B	265	LEU
1	B	314	GLU
1	B	464	ASN
1	B	647	ASP
1	A	78	GLY
1	A	433	ASN
1	A	670	GLY
1	B	674	GLY
1	A	529	ILE
1	A	627	GLY
1	A	722	GLY
1	B	198	PRO
1	B	227	PRO
1	A	147	VAL
1	A	366	ASN
1	A	383	ILE
1	B	466	GLY
1	B	467	ILE
1	B	595	ILE
1	B	383	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	671/710 (94%)	607 (90%)	64 (10%)	8 35
1	B	673/710 (95%)	607 (90%)	66 (10%)	8 34
All	All	1344/1420 (95%)	1214 (90%)	130 (10%)	8 34

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	35	HIS
1	A	42	HIS

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Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	LYS
1	A	51	GLU
1	A	52	GLU
1	A	56	LYS
1	A	85	ASP
1	A	93	SER
1	A	100	ASP
1	A	101	LYS
1	A	104	ILE
1	A	107	ILE
1	A	113	LEU
1	A	118	TYR
1	A	193	GLN
1	A	199	THR
1	A	211	ASN
1	A	233	LEU
1	A	239	GLU
1	A	241	PHE
1	A	259	LEU
1	A	283	ASP
1	A	292	LEU
1	A	321	ARG
1	A	329	PHE
1	A	333	GLU
1	A	343	ILE
1	A	346	ARG
1	A	373	LYS
1	A	381	LEU
1	A	404	ILE
1	A	426	SER
1	A	447	THR
1	A	449	THR
1	A	453	ASP
1	A	456	ASP
1	A	469	ASN
1	A	498	ARG
1	A	514	LEU
1	A	522	GLN
1	A	546	ASP
1	A	550	VAL
1	A	556	ASP

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Mol	Chain	Res	Type
1	A	574	LEU
1	A	578	LYS
1	A	586	ASN
1	A	594	ASN
1	A	601	LEU
1	A	604	ASN
1	A	611	GLN
1	A	619	THR
1	A	620	ASN
1	A	658	LEU
1	A	693	ASP
1	A	710	ASN
1	A	712	LYS
1	A	716	ASP
1	A	725	LEU
1	A	727	SER
1	A	737	PHE
1	A	764	GLN
1	A	772	PHE
1	B	28	ARG
1	B	32	GLN
1	B	36	LEU
1	B	60	GLU
1	B	62	LEU
1	B	92	ILE
1	B	105	LYS
1	B	107	ILE
1	B	111	ASP
1	B	128	VAL
1	B	131	ILE
1	B	136	ASP
1	B	140	ASN
1	B	178	LYS
1	B	193	GLN
1	B	197	HIS
1	B	199	THR
1	B	203	VAL
1	B	204	GLU
1	B	206	LEU
1	B	209	ASN
1	B	228	GLN
1	B	233	LEU

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Mol	Chain	Res	Type
1	B	235	LEU
1	B	242	ASN
1	B	250	GLN
1	B	282	SER
1	B	296	LEU
1	B	297	GLN
1	B	304	LYS
1	B	309	HIS
1	B	323	GLN
1	B	343	ILE
1	B	344	ASP
1	B	346	ARG
1	B	366	ASN
1	B	381	LEU
1	B	384	GLN
1	B	398	LEU
1	B	407	ASP
1	B	408	VAL
1	B	433	ASN
1	B	445	ASN
1	B	449	THR
1	B	456	ASP
1	B	464	ASN
1	B	475	PHE
1	B	487	ASP
1	B	496	ASN
1	B	503	ILE
1	B	516	ASN
1	B	523	ARG
1	B	533	GLN
1	B	556	ASP
1	B	571	ASN
1	B	580	THR
1	B	586	ASN
1	B	611	GLN
1	B	613	ASP
1	B	620	ASN
1	B	647	ASP
1	B	652	GLN
1	B	712	LYS
1	B	733	GLU
1	B	747	THR

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Mol	Chain	Res	Type
1	B	753	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	32	GLN
1	A	132	GLN
1	A	140	ASN
1	A	164	ASN
1	A	179	ASN
1	A	186	GLN
1	A	193	GLN
1	A	197	HIS
1	A	214	GLN
1	A	276	GLN
1	A	323	GLN
1	A	440	ASN
1	A	444	ASN
1	A	460	ASN
1	A	469	ASN
1	A	496	ASN
1	A	504	GLN
1	A	524	ASN
1	A	563	GLN
1	A	571	ASN
1	A	589	ASN
1	A	608	ASN
1	A	609	ASN
1	A	611	GLN
1	A	620	ASN
1	A	710	ASN
1	B	91	HIS
1	B	140	ASN
1	B	165	GLN
1	B	186	GLN
1	B	193	GLN
1	B	214	GLN
1	B	228	GLN
1	B	234	GLN
1	B	242	ASN
1	B	276	GLN

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Mol	Chain	Res	Type
1	B	277	HIS
1	B	342	GLN
1	B	366	ASN
1	B	390	GLN
1	B	440	ASN
1	B	445	ASN
1	B	496	ASN
1	B	516	ASN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	589	ASN
1	B	609	ASN
1	B	611	GLN
1	B	620	ASN
1	B	638	ASN
1	B	645	HIS
1	B	710	ASN
1	B	756	GLN
1	B	764	GLN
1	B	769	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	SD2	A	9002	2	32,33,33	0.96	1 (3%)	42,44,44	1.90	5 (11%)
3	SD2	B	9003	2	32,33,33	1.12	3 (9%)	42,44,44	2.27	7 (16%)

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	SD2	A	9002	2	-	5/32/44/44	0/2/2/2
3	SD2	B	9003	2	-	8/32/44/44	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9002	SD2	CBB-CBC	-3.62	1.37	1.51
3	B	9003	SD2	CBB-CBC	-3.42	1.38	1.51
3	B	9003	SD2	CAR-NAQ	2.24	1.51	1.47
3	B	9003	SD2	CBB-CAY	-2.03	1.48	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	9003	SD2	CAY-NAX-CAS	10.40	143.97	121.67
3	A	9002	SD2	CAY-NAX-CAS	7.46	137.67	121.67
3	A	9002	SD2	CBB-CAY-NAX	-5.44	99.87	110.88
3	B	9003	SD2	CAR-CAS-NAX	5.39	128.60	116.58
3	B	9003	SD2	CBB-CAY-NAX	4.70	120.38	110.88
3	A	9002	SD2	CAR-CAS-NAX	-4.56	106.44	116.58
3	A	9002	SD2	OAT-CAS-NAX	4.08	130.48	122.93
3	B	9003	SD2	OAT-CAS-NAX	-4.07	115.39	122.93
3	B	9003	SD2	CAS-CAR-NAQ	-2.59	105.42	112.56
3	A	9002	SD2	CBC-CBB-CAY	2.45	119.87	112.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	9003	SD2	CBB-CAY-CAZ	2.35	115.67	110.21
3	B	9003	SD2	CBE-SBD-CBC	2.10	107.61	100.40

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	9003	SD2	OAT-CAS-NAX-CAY
3	B	9003	SD2	CAR-CAS-NAX-CAY
3	B	9003	SD2	CBB-CAY-NAX-CAS
3	B	9003	SD2	CBB-CBC-SBD-CBE
3	B	9003	SD2	CAZ-CAY-CBB-CBC
3	A	9002	SD2	NAQ-CAR-CAS-NAX
3	B	9003	SD2	NAQ-CAR-CAS-NAX
3	A	9002	SD2	NAQ-CAR-CAS-OAT
3	B	9003	SD2	NAQ-CAR-CAS-OAT
3	A	9002	SD2	CAU-CAR-CAS-OAT
3	A	9002	SD2	CAU-CAR-CAS-NAX
3	A	9002	SD2	NAX-CAY-CBB-CBC
3	B	9003	SD2	CAG-CAF-NAA-CAB

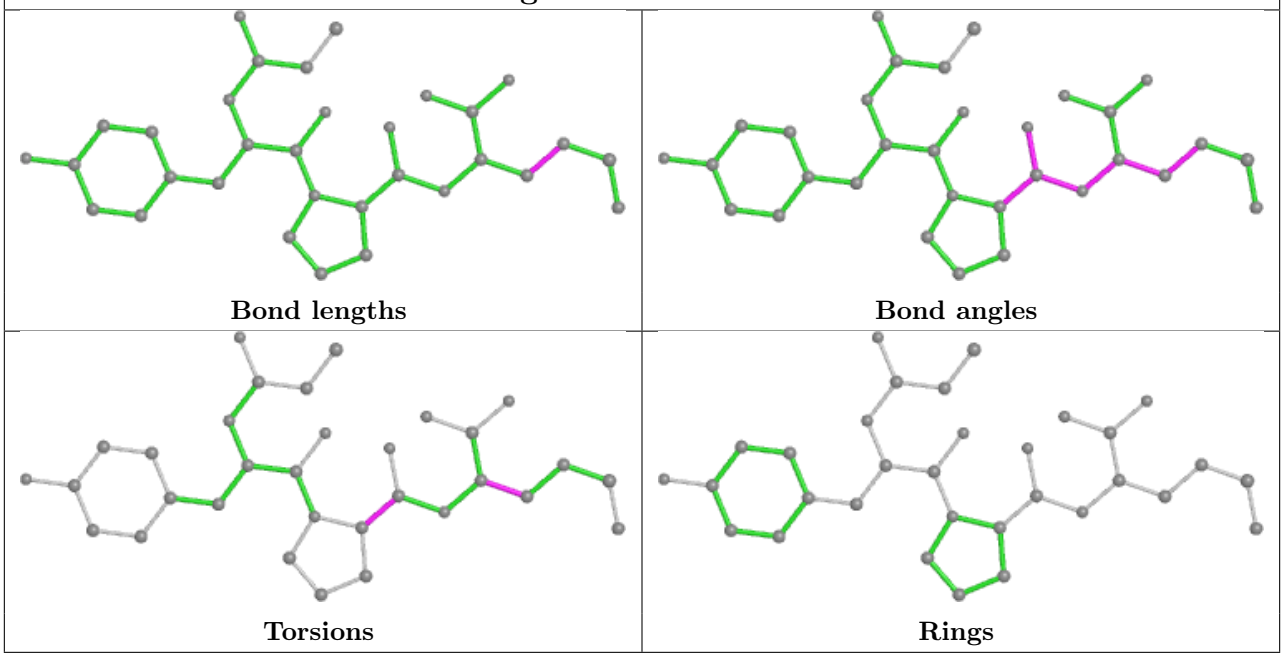
There are no ring outliers.

2 monomers are involved in 18 short contacts:

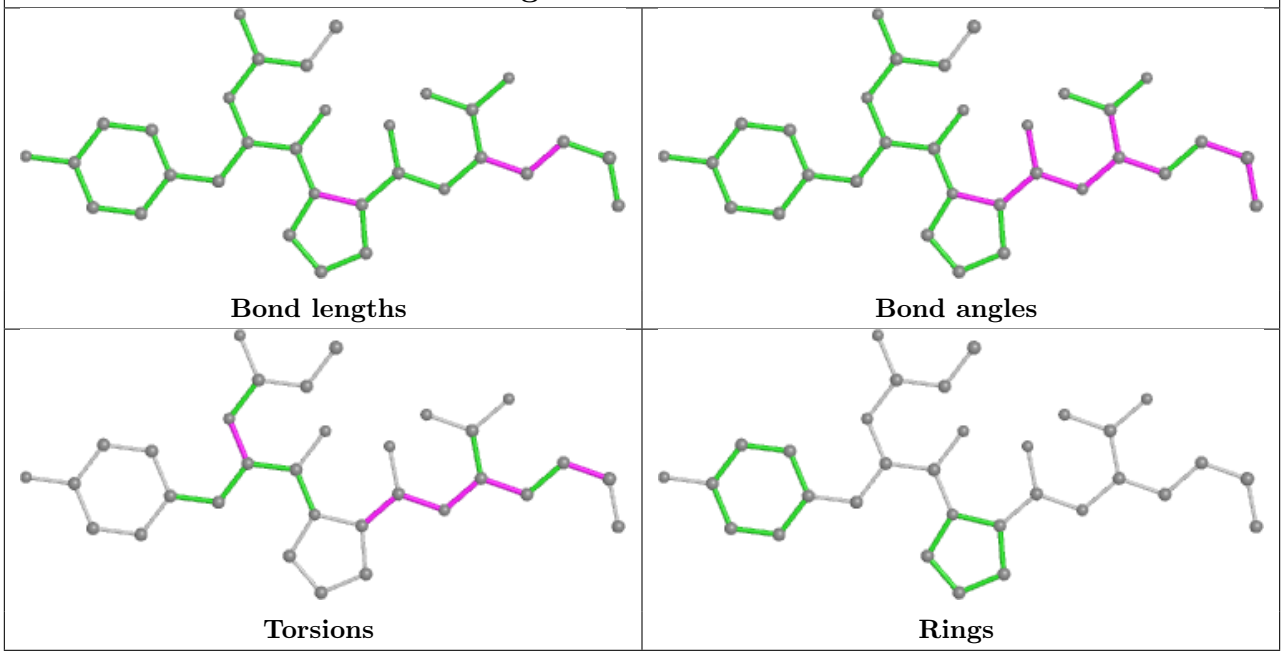
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9002	SD2	9	0
3	B	9003	SD2	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SD2 A 9002



Ligand SD2 B 9003



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	732/776 (94%)	-0.41	0 100 100	13, 39, 88, 93	0
1	B	734/776 (94%)	-0.42	1 (0%) 95 93	11, 38, 84, 96	0
All	All	1466/1552 (94%)	-0.41	1 (0%) 95 93	11, 38, 86, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LYS	2.3

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

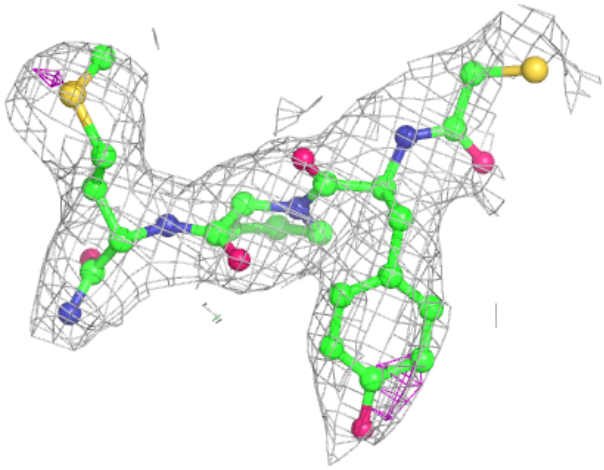
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

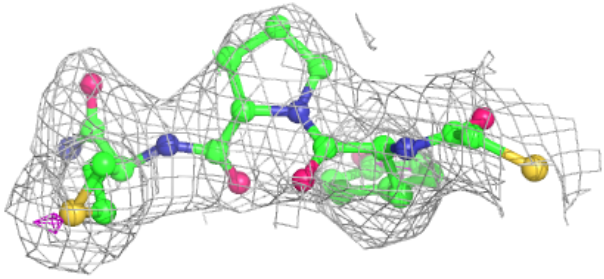
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SD2	A	9002	32/32	0.96	0.25	21,23,30,41	0
3	SD2	B	9003	32/32	0.96	0.23	16,23,32,37	0
2	ZN	A	9001	1/1	0.99	0.12	21,21,21,21	0
2	ZN	B	9002	1/1	0.99	0.12	17,17,17,17	0

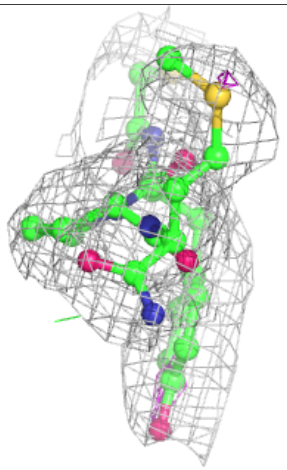
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SD2 A 9002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

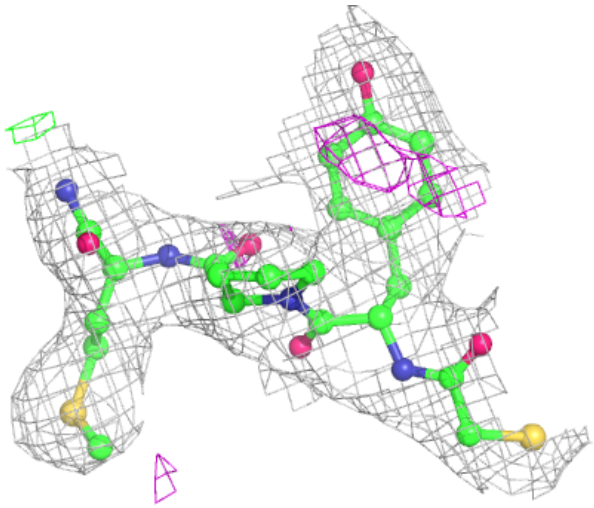


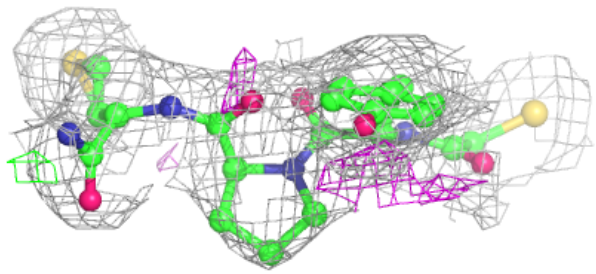


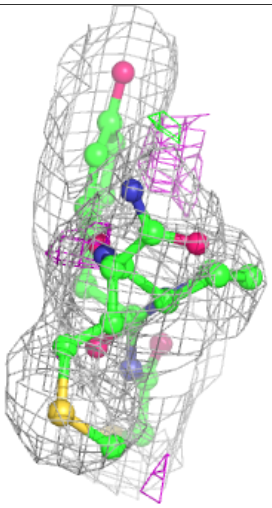


Electron density around SD2 B 9003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.