



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:50 PM GMT

PDB ID : 1M8P
Title : Crystal Structure of *P. chrysogenum* ATP Sulfurylase in the T-state
Authors : MacRae, I.J.; Segel, I.H.; Fisher, A.J.
Deposited on : 2002-07-25
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

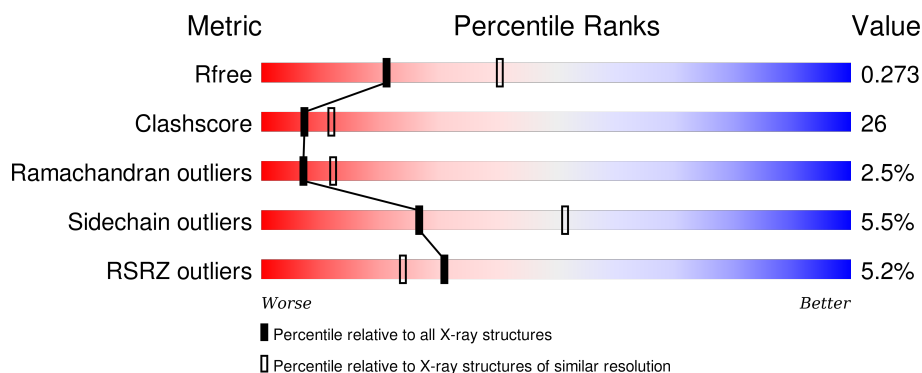
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

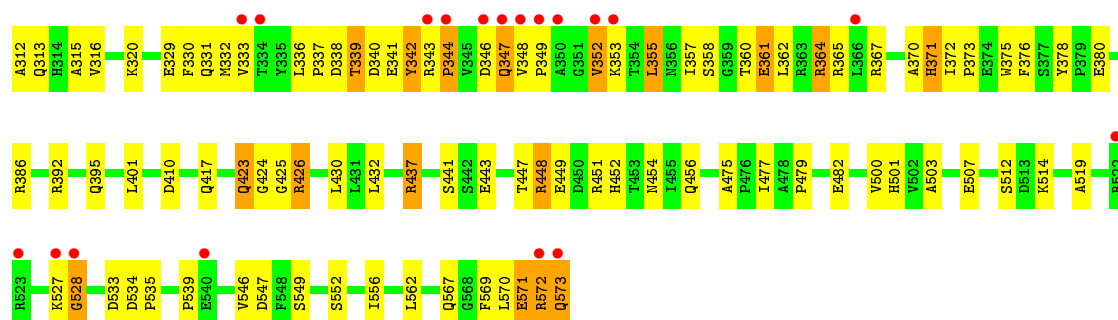
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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	573	<div> <div>8%</div> <div> <div></div> <div>51%</div> <div>42%</div> <div>7%</div> </div> </div>
1	B	573	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>5%</div> </div> </div>
1	C	573	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>33%</div> <div>.</div> </div> </div>

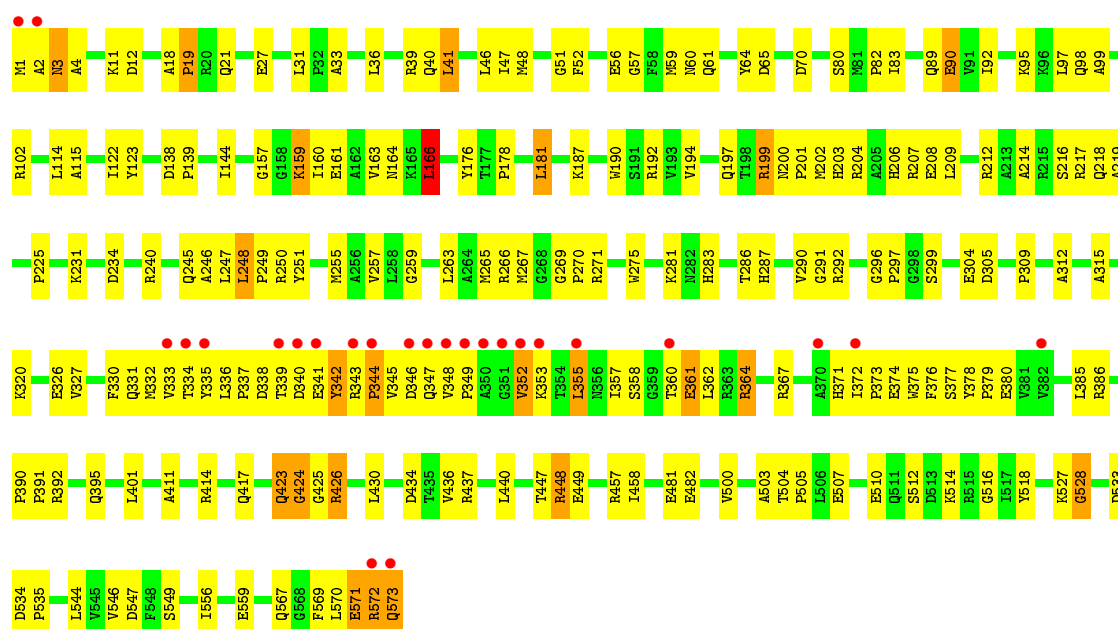
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	13	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	13	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	13	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	162	Total	O	0	0
			162	162		
3	C	196	Total	O	0	0
			196	196		



- Molecule 1: sulfate adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.45Å 135.45Å 234.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.33 – 2.60 29.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.33-2.60) 99.2 (29.33-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.272 0.218 , 0.273	Depositor DCC
R_{free} test set	3968 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.9	EDS
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 85986 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14054	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.44 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.8300e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PPS

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	0.52	1/4596 (0.0%)	0.75	1/6227 (0.0%)
1	B	0.58	0/4596	0.79	1/6227 (0.0%)
1	C	0.60	0/4596	0.81	4/6227 (0.1%)
All	All	0.57	1/13788 (0.0%)	0.78	6/18681 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	565	GLU	CG-CD	5.08	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	C	41	LEU	CA-CB-CG	-5.77	102.03	115.30
1	B	424	GLY	N-CA-C	5.67	127.27	113.10
1	C	166	LEU	CA-CB-CG	5.57	128.10	115.30
1	C	424	GLY	N-CA-C	5.35	126.47	113.10
1	A	424	GLY	N-CA-C	5.30	126.36	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4501	0	4450	275	0
1	B	4501	0	4450	213	0
1	C	4501	0	4450	211	0
2	A	31	0	11	2	0
2	B	31	0	12	4	0
2	C	31	0	11	2	0
3	A	100	0	0	8	0
3	B	162	0	0	11	0
3	C	196	0	0	14	0
All	All	14054	0	13384	699	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 26.

All (699) 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:C:337:PRO:HD2	1:C:353:LYS:HB2	1.34	1.08
1:A:337:PRO:HD2	1:A:353:LYS:HB2	1.36	1.05
1:B:337:PRO:HD2	1:B:353:LYS:HB2	1.37	1.04
1:C:481:GLU:HG3	3:C:647:HOH:O	1.61	0.99
1:B:423:GLN:HE21	1:B:425:GLY:H	1.08	0.99
1:B:423:GLN:NE2	1:B:425:GLY:H	1.61	0.99
1:B:48:MET:CE	1:B:115:ALA:HB2	1.93	0.98
1:C:358:SER:HB3	1:C:361:GLU:HB2	1.45	0.97
1:B:1:MET:HG2	1:B:2:ALA:H	1.31	0.96
1:B:358:SER:HB3	1:B:361:GLU:HB2	1.50	0.94
1:A:358:SER:HB3	1:A:361:GLU:HB2	1.50	0.94
1:A:192:ARG:HA	1:A:286:THR:HG21	1.50	0.93
1:A:423:GLN:NE2	1:A:425:GLY:H	1.65	0.93
1:C:423:GLN:NE2	1:C:425:GLY:H	1.68	0.91
1:A:92:ILE:HA	1:A:97:LEU:HD12	1.53	0.90
1:B:231:LYS:HB2	1:B:234:ASP:HB2	1.53	0.89
1:A:401:LEU:HD23	1:A:500:VAL:HB	1.51	0.89
1:B:401:LEU:HD23	1:B:500:VAL:HB	1.53	0.89
1:C:337:PRO:HD2	1:C:353:LYS:CB	2.03	0.89
1:C:200:ASN:HB3	1:C:201:PRO:HD2	1.54	0.88
1:B:192:ARG:HB2	1:B:192:ARG:HH11	1.39	0.87
1:C:59:MET:HE3	1:C:64:TYR:HA	1.55	0.87
1:C:401:LEU:HD23	1:C:500:VAL:HB	1.55	0.86
1:B:337:PRO:HD2	1:B:353:LYS:CB	2.05	0.86
1:A:423:GLN:HE21	1:A:425:GLY:H	1.17	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PRO:HD2	1:A:353:LYS:CB	2.05	0.86
1:C:114:LEU:HD13	1:C:166:LEU:HD22	1.55	0.85
1:A:300:ASN:HD21	1:A:304:GLU:HB2	1.41	0.85
1:C:208:GLU:O	1:C:212:ARG:HG2	1.75	0.85
1:A:60:ASN:HB2	1:A:121:ASP:OD2	1.77	0.85
1:A:11:LYS:HD3	1:A:54:PRO:HA	1.57	0.84
1:C:373:PRO:HB3	1:C:375:TRP:NE1	1.93	0.84
1:A:300:ASN:ND2	1:A:304:GLU:HB2	1.92	0.83
1:C:423:GLN:HE21	1:C:425:GLY:H	1.21	0.83
1:A:165:LYS:O	1:A:166:LEU:HB3	1.77	0.83
1:B:202:MET:N	3:B:610:HOH:O	2.12	0.82
1:B:286:THR:OG1	1:B:287:HIS:HD2	1.64	0.81
1:B:200:ASN:HB3	1:B:201:PRO:HD2	1.63	0.80
1:C:11:LYS:HE2	1:C:56:GLU:OE2	1.81	0.80
1:C:61:GLN:HG3	1:C:123:TYR:CD1	2.16	0.80
1:B:159:LYS:NZ	3:B:578:HOH:O	2.12	0.79
1:B:373:PRO:HB3	1:B:375:TRP:NE1	1.97	0.78
1:A:31:LEU:HD22	1:A:102:ARG:HB3	1.65	0.78
1:C:192:ARG:NH1	1:C:217:ARG:O	2.17	0.78
1:C:200:ASN:HB3	1:C:201:PRO:CD	2.14	0.77
1:B:61:GLN:HG3	1:B:123:TYR:CG	2.21	0.76
1:A:373:PRO:HB3	1:A:375:TRP:NE1	2.01	0.76
1:A:131:ALA:HB2	1:A:147:LEU:HD23	1.65	0.76
1:B:48:MET:HE3	1:B:115:ALA:HB2	1.67	0.75
1:A:37:THR:OG1	1:A:40:GLN:HG3	1.87	0.74
1:B:59:MET:HE1	1:B:82:PRO:HA	1.69	0.74
1:A:344:PRO:HB2	1:A:347:GLN:HG2	1.69	0.74
1:B:61:GLN:HG3	1:B:123:TYR:CD2	2.22	0.74
1:A:199:ARG:HB3	1:A:265:MET:HE1	1.70	0.74
1:A:401:LEU:CD2	1:A:500:VAL:HB	2.18	0.73
1:B:423:GLN:NE2	1:B:425:GLY:N	2.36	0.73
1:C:570:LEU:O	1:C:572:ARG:N	2.21	0.73
1:A:204:ARG:HD3	1:A:378:TYR:CZ	2.24	0.73
1:C:336:LEU:HD22	1:C:352:VAL:HG11	1.70	0.72
1:B:300:ASN:ND2	1:B:304:GLU:HB2	2.04	0.72
1:C:12:ASP:HB3	3:C:663:HOH:O	1.89	0.72
1:B:401:LEU:CD2	1:B:500:VAL:HB	2.19	0.72
1:B:357:ILE:HD11	1:B:373:PRO:HG2	1.72	0.71
1:A:147:LEU:HA	1:A:151:VAL:CG2	2.21	0.71
1:C:392:ARG:HG3	1:C:392:ARG:HH11	1.55	0.71
1:B:344:PRO:HB2	1:B:347:GLN:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:HA	1:A:157:GLY:HA3	1.71	0.70
1:C:286:THR:OG1	1:C:287:HIS:HD2	1.74	0.70
1:A:47:ILE:HD11	1:A:83:ILE:HG21	1.73	0.70
1:A:423:GLN:NE2	1:A:425:GLY:N	2.38	0.70
1:A:570:LEU:O	1:A:572:ARG:N	2.23	0.70
1:C:204:ARG:HB3	1:C:376:PHE:O	1.91	0.70
1:C:331:GLN:HE21	1:C:344:PRO:HB3	1.57	0.70
1:C:33:ALA:O	1:C:95:LYS:HE2	1.92	0.70
1:A:140:GLU:OE2	1:A:300:ASN:HB2	1.92	0.69
1:B:331:GLN:HE21	1:B:344:PRO:HB3	1.56	0.69
1:B:247:LEU:HD12	1:B:247:LEU:O	1.92	0.69
1:C:344:PRO:HB2	1:C:347:GLN:HG2	1.73	0.69
1:A:131:ALA:O	1:A:144:ILE:HD11	1.93	0.69
1:C:357:ILE:HD11	1:C:373:PRO:HG2	1.74	0.69
1:A:331:GLN:HE21	1:A:344:PRO:HB3	1.58	0.69
1:A:352:VAL:O	1:A:353:LYS:HG2	1.93	0.69
1:B:1:MET:HG2	1:B:2:ALA:N	2.04	0.69
1:A:28:ALA:HA	1:A:31:LEU:HD12	1.74	0.69
1:B:59:MET:CE	1:B:82:PRO:HA	2.23	0.69
1:A:202:MET:HA	1:A:206:HIS:ND1	2.08	0.69
1:C:3:ASN:HA	3:C:634:HOH:O	1.92	0.68
1:C:401:LEU:CD2	1:C:500:VAL:HB	2.22	0.68
1:A:102:ARG:HH11	1:A:116:ILE:HG21	1.58	0.68
1:A:59:MET:CE	1:A:67:VAL:HG21	2.24	0.68
1:A:357:ILE:HD11	1:A:373:PRO:HG2	1.74	0.68
1:B:570:LEU:O	1:B:572:ARG:N	2.27	0.68
1:C:449:GLU:HG3	3:C:677:HOH:O	1.93	0.68
1:B:336:LEU:HD22	1:B:352:VAL:HG11	1.76	0.68
1:B:395:GLN:O	1:B:426:ARG:NH1	2.27	0.68
1:C:528:GLY:HA2	1:C:533:ASP:HB2	1.75	0.68
1:B:200:ASN:HB3	1:B:201:PRO:CD	2.24	0.67
1:C:345:VAL:CG1	3:C:693:HOH:O	2.42	0.67
1:A:129:LYS:HE2	1:A:133:LEU:HD11	1.76	0.67
1:C:204:ARG:CZ	1:C:342:TYR:OH	2.42	0.67
1:A:392:ARG:HG3	1:A:392:ARG:HH11	1.57	0.67
1:B:372:ILE:HG13	1:B:386:ARG:HH22	1.58	0.67
1:C:4:ALA:O	1:C:281:LYS:HE2	1.93	0.67
1:A:565:GLU:HG2	3:A:655:HOH:O	1.93	0.67
1:A:313:GLN:HB3	1:A:329:GLU:HG2	1.75	0.67
1:B:117:LEU:C	1:B:117:LEU:HD23	2.14	0.67
1:C:423:GLN:NE2	1:C:425:GLY:N	2.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:GLY:HA2	1:B:533:ASP:HB2	1.77	0.67
1:A:90:GLU:O	1:A:94:GLU:HB2	1.93	0.67
1:C:337:PRO:HG3	1:C:355:LEU:HD12	1.77	0.67
1:A:193:VAL:H	1:A:286:THR:HG23	1.58	0.67
1:A:344:PRO:HD2	1:A:347:GLN:HG3	1.77	0.67
1:C:217:ARG:HG2	1:C:217:ARG:HH11	1.58	0.67
1:B:352:VAL:O	1:B:353:LYS:HG2	1.94	0.66
1:B:231:LYS:HB2	1:B:234:ASP:CB	2.22	0.66
1:B:449:GLU:HG3	3:B:623:HOH:O	1.95	0.66
1:A:527:LYS:HG2	1:A:528:GLY:N	2.11	0.66
1:A:426:ARG:NH2	1:A:569:PHE:O	2.28	0.66
1:A:337:PRO:HG3	1:A:355:LEU:HD12	1.77	0.66
1:C:352:VAL:O	1:C:353:LYS:HG2	1.95	0.66
1:A:572:ARG:HD2	1:B:253:ASN:HB3	1.78	0.66
1:C:212:ARG:HH21	1:C:342:TYR:HB2	1.61	0.65
1:A:221:VAL:HB	1:A:256:ALA:HB2	1.78	0.65
1:B:313:GLN:HG3	3:B:584:HOH:O	1.95	0.65
1:A:33:ALA:O	1:A:95:LYS:HE2	1.97	0.65
1:C:320:LYS:HE3	1:C:326:GLU:HA	1.77	0.65
1:C:59:MET:CE	1:C:64:TYR:HA	2.27	0.65
1:C:57:GLY:HA2	1:C:160:ILE:HG12	1.78	0.65
1:B:90:GLU:O	1:B:94:GLU:HB2	1.96	0.65
1:A:131:ALA:HB1	1:A:144:ILE:HG13	1.79	0.65
1:A:336:LEU:HD22	1:A:352:VAL:HG11	1.77	0.65
1:A:302:LYS:HE3	1:A:304:GLU:OE2	1.97	0.64
1:C:291:GLY:HA3	1:C:330:PHE:CE2	2.32	0.64
1:C:57:GLY:HA2	1:C:160:ILE:CG1	2.27	0.64
1:A:395:GLN:O	1:A:426:ARG:NH1	2.31	0.64
1:C:372:ILE:HG13	1:C:386:ARG:HH22	1.62	0.64
1:B:337:PRO:HG3	1:B:355:LEU:HD12	1.80	0.64
1:A:27:GLU:OE2	1:A:102:ARG:HD3	1.97	0.64
1:A:343:ARG:HB3	1:A:347:GLN:HB2	1.81	0.63
1:C:395:GLN:O	1:C:426:ARG:NH1	2.30	0.63
1:C:115:ALA:HA	1:C:163:VAL:HG13	1.81	0.63
1:A:231:LYS:HB2	1:A:234:ASP:HB2	1.79	0.63
1:B:546:VAL:HG11	1:B:556:ILE:CG2	2.29	0.63
1:B:549:SER:O	3:B:716:HOH:O	2.15	0.63
1:B:527:LYS:HG2	1:B:528:GLY:N	2.12	0.63
1:C:527:LYS:HG2	1:C:528:GLY:N	2.14	0.62
1:C:331:GLN:NE2	1:C:344:PRO:HB3	2.15	0.62
1:C:343:ARG:HB3	1:C:347:GLN:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ARG:HH11	1:B:392:ARG:HG3	1.65	0.62
1:C:546:VAL:HG11	1:C:556:ILE:HD13	1.81	0.62
1:C:344:PRO:HD2	1:C:347:GLN:HG3	1.81	0.62
1:B:331:GLN:NE2	1:B:344:PRO:HB3	2.14	0.62
1:A:48:MET:HE3	1:A:162:ALA:HA	1.80	0.62
1:B:199:ARG:HD2	1:B:265:MET:CE	2.29	0.62
1:B:55:LEU:HD12	1:B:56:GLU:N	2.14	0.62
1:B:344:PRO:HD2	1:B:347:GLN:HG3	1.82	0.62
1:A:272:GLU:O	1:A:275:TRP:HB3	2.00	0.62
1:B:207:ARG:O	1:B:211:VAL:HG23	2.00	0.62
1:C:159:LYS:NZ	3:C:578:HOH:O	2.32	0.61
1:B:343:ARG:HB3	1:B:347:GLN:HB2	1.82	0.61
1:B:55:LEU:HD11	1:B:57:GLY:O	2.00	0.61
1:B:333:VAL:HB	1:B:343:ARG:C	2.21	0.61
1:C:434:ASP:HB3	2:C:576:PPS:O3P	1.99	0.61
1:C:372:ILE:HG13	1:C:386:ARG:NH2	2.15	0.61
1:A:372:ILE:HG13	1:A:386:ARG:HH22	1.65	0.61
1:B:300:ASN:HD21	1:B:304:GLU:HB2	1.65	0.61
1:B:534:ASP:OD2	1:B:535:PRO:HD2	2.01	0.61
1:A:528:GLY:HA2	1:A:533:ASP:HB2	1.82	0.61
1:C:60:ASN:HA	1:C:157:GLY:HA3	1.82	0.61
1:B:209:LEU:CD1	1:B:330:PHE:HB2	2.32	0.60
1:A:147:LEU:HA	1:A:151:VAL:HG23	1.81	0.60
1:C:333:VAL:HB	1:C:343:ARG:C	2.21	0.60
1:C:345:VAL:HG13	3:C:693:HOH:O	2.00	0.60
1:C:426:ARG:NH2	1:C:569:PHE:O	2.34	0.60
1:A:199:ARG:HH11	1:A:265:MET:CE	2.15	0.60
1:A:331:GLN:NE2	1:A:344:PRO:HB3	2.16	0.59
1:C:546:VAL:HG11	1:C:556:ILE:CG2	2.32	0.59
1:C:204:ARG:HD3	1:C:378:TYR:CZ	2.37	0.59
1:A:27:GLU:O	1:A:31:LEU:HG	2.03	0.59
1:A:192:ARG:CD	1:A:218:GLN:O	2.51	0.59
1:B:372:ILE:HG13	1:B:386:ARG:NH2	2.16	0.59
1:A:131:ALA:HB1	1:A:144:ILE:CG1	2.33	0.59
1:B:250:ARG:NH2	1:B:380:GLU:OE2	2.35	0.59
1:A:165:LYS:O	1:A:166:LEU:CB	2.45	0.59
1:B:339:THR:HG22	1:B:341:GLU:OE2	2.03	0.58
1:B:199:ARG:HH11	1:B:265:MET:HE1	1.67	0.58
1:C:18:ALA:HB3	1:C:19:PRO:HD3	1.86	0.58
1:C:187:LYS:HE3	3:C:758:HOH:O	2.01	0.58
1:A:122:ILE:O	1:A:122:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:HD11	1:A:275:TRP:CH2	2.38	0.58
1:A:546:VAL:HG11	1:A:556:ILE:HD13	1.85	0.58
1:A:102:ARG:NH1	1:A:116:ILE:HG21	2.17	0.58
1:A:226:VAL:O	1:A:240:ARG:NH2	2.37	0.58
2:A:574:PPS:H5'2	2:A:574:PPS:N3	2.19	0.58
1:A:199:ARG:NH1	1:A:265:MET:HE3	2.19	0.58
1:C:392:ARG:HG3	1:C:392:ARG:NH1	2.18	0.58
1:C:373:PRO:HB3	1:C:375:TRP:CD1	2.39	0.58
1:B:55:LEU:HD12	1:B:56:GLU:H	1.69	0.58
1:C:138:ASP:O	1:C:144:ILE:HD12	2.04	0.58
1:A:333:VAL:HB	1:A:343:ARG:C	2.25	0.57
1:A:123:TYR:O	1:A:154:PHE:HB3	2.04	0.57
1:A:272:GLU:HG3	1:A:275:TRP:HE3	1.69	0.57
1:B:546:VAL:HG11	1:B:556:ILE:HD13	1.86	0.57
1:A:572:ARG:NH2	3:A:651:HOH:O	2.37	0.57
1:A:73:LEU:HG	1:A:79:PHE:CB	2.34	0.57
1:B:240:ARG:HD2	1:B:244:TYR:CE1	2.38	0.57
1:A:144:ILE:HG22	1:A:145:VAL:N	2.19	0.57
1:B:194:VAL:HG22	1:B:287:HIS:HB2	1.87	0.57
1:C:231:LYS:HB2	1:C:234:ASP:HB2	1.85	0.57
1:A:344:PRO:HD2	1:A:347:GLN:CG	2.35	0.57
1:A:392:ARG:HG3	1:A:392:ARG:NH1	2.20	0.57
1:A:125:PRO:HD2	1:A:154:PHE:HA	1.87	0.57
1:A:250:ARG:HD2	1:A:378:TYR:CE2	2.40	0.57
1:A:147:LEU:HA	1:A:151:VAL:HG21	1.85	0.57
1:C:59:MET:HB2	1:C:83:ILE:O	2.05	0.56
1:A:192:ARG:HA	1:A:286:THR:CG2	2.29	0.56
1:C:546:VAL:CG1	1:C:556:ILE:HD13	2.35	0.56
1:C:339:THR:HG22	1:C:341:GLU:OE2	2.06	0.56
1:A:129:LYS:HG2	1:A:133:LEU:HD11	1.87	0.56
1:A:287:HIS:ND1	1:A:326:GLU:HB2	2.20	0.56
1:B:201:PRO:O	1:B:202:MET:HB2	2.06	0.56
1:A:204:ARG:HD3	1:A:378:TYR:OH	2.06	0.56
1:A:194:VAL:HG22	1:A:287:HIS:HB2	1.87	0.56
1:A:546:VAL:HG11	1:A:556:ILE:CG2	2.36	0.56
1:B:199:ARG:HD2	1:B:265:MET:HE3	1.88	0.56
1:B:199:ARG:HH11	1:B:265:MET:CE	2.18	0.56
1:B:57:GLY:HA2	1:B:160:ILE:HG12	1.87	0.56
1:B:18:ALA:O	1:B:21:GLN:HB2	2.06	0.55
1:A:423:GLN:HE22	1:A:425:GLY:HA3	1.70	0.55
1:C:214:ALA:HB1	1:C:219:ALA:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ALA:HB3	1:C:255:MET:HE2	1.87	0.55
1:C:417:GLN:OE1	1:C:430:LEU:HD22	2.07	0.55
1:B:451:ARG:NH2	2:B:575:PPS:N1	2.51	0.55
1:A:207:ARG:O	1:A:207:ARG:HD3	2.07	0.55
1:A:339:THR:HG22	1:A:341:GLU:OE2	2.06	0.55
1:C:336:LEU:HD22	1:C:352:VAL:CG1	2.35	0.55
1:A:527:LYS:HG2	1:A:528:GLY:H	1.70	0.55
1:A:86:ASP:OD2	1:A:152:LYS:HG2	2.06	0.55
1:C:336:LEU:O	1:C:340:ASP:N	2.31	0.55
1:C:199:ARG:HH11	1:C:265:MET:HE3	1.71	0.55
1:B:159:LYS:HE2	1:B:159:LYS:N	2.21	0.55
1:A:192:ARG:HD3	1:A:218:GLN:O	2.07	0.54
1:A:546:VAL:CG1	1:A:556:ILE:HD13	2.38	0.54
1:A:190:TRP:CZ3	1:A:257:VAL:HG23	2.43	0.54
1:C:27:GLU:O	1:C:31:LEU:HG	2.08	0.54
1:B:21:GLN:NE2	1:B:163:VAL:O	2.40	0.54
1:B:546:VAL:CG1	1:B:556:ILE:HD13	2.37	0.54
1:A:59:MET:HE1	1:A:67:VAL:HG21	1.88	0.54
1:C:199:ARG:HB3	1:C:265:MET:CE	2.38	0.54
1:C:59:MET:HE3	1:C:64:TYR:CA	2.31	0.54
1:B:286:THR:OG1	1:B:287:HIS:CD2	2.53	0.54
1:B:123:TYR:CE1	1:B:155:TYR:HB2	2.43	0.54
1:C:330:PHE:C	1:C:330:PHE:CD1	2.81	0.54
1:B:80:SER:HB2	1:B:271:ARG:HD3	1.90	0.54
1:C:201:PRO:O	1:C:202:MET:HB2	2.06	0.54
1:B:373:PRO:HB3	1:B:375:TRP:CD1	2.42	0.53
1:B:185:PHE:O	1:B:190:TRP:HB2	2.08	0.53
1:A:331:GLN:O	1:A:331:GLN:HG3	2.08	0.53
1:B:331:GLN:O	1:B:331:GLN:HG3	2.08	0.53
1:A:372:ILE:HG13	1:A:386:ARG:NH2	2.22	0.53
1:A:292:ARG:NH2	1:A:309:PRO:HB3	2.23	0.53
1:B:192:ARG:HH11	1:B:192:ARG:CB	2.17	0.53
1:B:60:ASN:HB2	1:B:121:ASP:OD2	2.07	0.53
1:C:199:ARG:HB3	1:C:265:MET:HE1	1.91	0.53
1:C:204:ARG:HD3	1:C:378:TYR:CE1	2.44	0.53
1:B:199:ARG:NH1	1:B:265:MET:CE	2.71	0.53
1:B:432:LEU:HD23	1:B:475:ALA:HB3	1.89	0.53
1:B:209:LEU:HD11	1:B:330:PHE:HB2	1.89	0.53
1:C:212:ARG:NH2	1:C:342:TYR:CD1	2.77	0.53
1:C:344:PRO:HD2	1:C:347:GLN:CG	2.38	0.53
1:B:214:ALA:HB1	1:B:219:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:TYR:CD2	1:B:181:LEU:HD13	2.43	0.53
1:C:331:GLN:HG3	1:C:331:GLN:O	2.08	0.53
1:B:423:GLN:HE21	1:B:425:GLY:N	1.91	0.53
1:B:18:ALA:HB3	1:B:19:PRO:HD3	1.91	0.53
1:B:101:SER:HB2	1:B:119:ILE:HD12	1.90	0.53
1:B:223:ILE:HG22	1:B:225:PRO:HD3	1.90	0.53
1:B:59:MET:HE2	1:B:83:ILE:H	1.74	0.52
1:B:426:ARG:NH2	1:B:569:PHE:O	2.42	0.52
1:A:336:LEU:HB2	1:A:339:THR:HB	1.90	0.52
1:C:250:ARG:NE	1:C:378:TYR:CD2	2.77	0.52
1:B:107:ASP:HB2	1:B:114:LEU:HD11	1.92	0.52
1:A:176:TYR:CG	1:A:181:LEU:HD13	2.45	0.52
1:C:336:LEU:HB2	1:C:339:THR:HB	1.92	0.52
1:C:342:TYR:CD1	1:C:342:TYR:N	2.77	0.52
1:A:22:ALA:O	1:A:25:ALA:HB3	2.09	0.52
1:B:527:LYS:HG2	1:B:528:GLY:H	1.73	0.52
1:A:275:TRP:O	1:A:279:ILE:HG13	2.10	0.52
1:C:570:LEU:O	1:C:571:GLU:C	2.48	0.52
1:A:48:MET:CE	1:A:162:ALA:HA	2.40	0.52
1:B:2:ALA:HA	3:B:617:HOH:O	2.09	0.52
1:A:140:GLU:CD	1:A:300:ASN:HB2	2.30	0.52
1:B:90:GLU:N	1:B:90:GLU:OE1	2.35	0.52
1:B:272:GLU:HG2	1:B:276:HIS:NE2	2.24	0.52
1:A:281:LYS:HB2	1:A:325:ILE:HD12	1.92	0.52
1:A:330:PHE:C	1:A:330:PHE:CD1	2.83	0.52
1:C:336:LEU:HD11	1:C:343:ARG:HD2	1.92	0.52
1:A:373:PRO:HB3	1:A:375:TRP:CD1	2.45	0.52
1:B:336:LEU:HD22	1:B:352:VAL:CG1	2.40	0.52
1:B:297:PRO:HB2	1:B:306:PHE:CD1	2.44	0.52
1:B:330:PHE:C	1:B:330:PHE:CD1	2.83	0.52
1:A:423:GLN:HE21	1:A:425:GLY:N	1.98	0.51
1:A:291:GLY:HA3	1:A:330:PHE:CE2	2.44	0.51
1:C:194:VAL:HA	1:C:287:HIS:HB2	1.93	0.51
1:A:107:ASP:HB2	1:A:114:LEU:HD11	1.92	0.51
1:C:207:ARG:HD3	1:C:207:ARG:O	2.10	0.51
1:B:546:VAL:HG11	1:B:556:ILE:HG23	1.92	0.51
1:A:48:MET:HE2	1:A:162:ALA:CB	2.40	0.51
1:A:132:LYS:HA	1:A:137:GLY:HA2	1.92	0.51
1:C:423:GLN:HE22	1:C:425:GLY:HA3	1.76	0.51
1:A:92:ILE:HD11	1:A:154:PHE:CD1	2.45	0.51
1:A:441:SER:OG	1:A:454:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ARG:NH2	1:C:342:TYR:HB2	2.24	0.51
1:B:93:ASP:O	1:B:95:LYS:N	2.44	0.51
1:B:95:LYS:O	1:B:96:LYS:HB2	2.11	0.51
1:B:57:GLY:HA2	1:B:160:ILE:CG1	2.40	0.51
1:C:516:GLY:HA2	3:C:595:HOH:O	2.10	0.51
1:A:342:TYR:CD1	1:A:342:TYR:N	2.78	0.51
1:B:344:PRO:HD2	1:B:347:GLN:CG	2.39	0.51
1:B:121:ASP:OD1	1:B:123:TYR:CD2	2.64	0.51
1:B:166:LEU:H	1:B:166:LEU:HD12	1.76	0.51
1:B:102:ARG:NH2	1:B:161:GLU:OE1	2.44	0.51
1:B:342:TYR:CD1	1:B:342:TYR:N	2.78	0.50
1:B:60:ASN:HA	1:B:157:GLY:HA3	1.93	0.50
1:A:86:ASP:HB2	1:A:152:LYS:HB2	1.94	0.50
1:A:200:ASN:HB3	1:A:201:PRO:HD2	1.93	0.50
1:B:392:ARG:NH1	1:B:392:ARG:HG3	2.27	0.50
1:A:114:LEU:O	1:A:163:VAL:HG13	2.11	0.50
1:B:477:ILE:HG22	1:B:479:PRO:HG3	1.93	0.50
1:C:204:ARG:NH1	1:C:204:ARG:HG2	2.26	0.50
1:B:425:GLY:HA2	1:B:573:GLN:HE22	1.77	0.50
1:A:140:GLU:O	1:A:141:HIS:C	2.50	0.50
1:C:3:ASN:ND2	3:C:634:HOH:O	2.44	0.50
1:A:330:PHE:HD1	1:A:332:MET:H	1.59	0.50
1:A:119:ILE:HG22	1:A:120:ASP:N	2.26	0.50
1:A:534:ASP:OD2	1:A:535:PRO:HD2	2.12	0.50
1:B:552:SER:O	1:B:556:ILE:HG13	2.11	0.50
1:A:57:GLY:HA3	1:A:159:LYS:HA	1.93	0.50
1:B:337:PRO:HG2	1:B:355:LEU:HG	1.94	0.50
1:C:61:GLN:HG3	1:C:123:TYR:CE1	2.47	0.50
1:A:73:LEU:HG	1:A:79:PHE:HB2	1.93	0.50
1:C:225:PRO:HD2	1:C:259:GLY:O	2.12	0.50
1:C:330:PHE:HD1	1:C:332:MET:H	1.60	0.50
1:A:417:GLN:OE1	1:A:430:LEU:HD22	2.12	0.50
1:C:178:PRO:HG3	1:C:283:HIS:CE1	2.46	0.50
1:B:65:ASP:O	1:B:69:GLU:HG2	2.12	0.49
1:B:43:ASP:O	1:B:47:ILE:HG13	2.11	0.49
1:A:436:VAL:HG11	1:A:458:ILE:HD11	1.94	0.49
1:B:52:PHE:O	1:B:53:SER:C	2.51	0.49
1:A:160:ILE:CG2	1:A:161:GLU:N	2.74	0.49
1:A:336:LEU:HD11	1:A:343:ARG:HD2	1.94	0.49
1:B:336:LEU:HB2	1:B:339:THR:HB	1.92	0.49
1:A:36:LEU:HB3	1:A:40:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD23	1:A:280:ARG:NH2	2.27	0.49
1:C:299:SER:HB2	1:C:304:GLU:O	2.11	0.49
1:B:417:GLN:OE1	1:B:430:LEU:HD22	2.12	0.49
1:A:388:SER:HB3	3:A:642:HOH:O	2.11	0.49
1:B:336:LEU:HD11	1:B:343:ARG:HD2	1.95	0.49
1:A:361:GLU:O	1:A:365:ARG:HG3	2.12	0.49
1:B:360:THR:O	1:B:364:ARG:HB2	2.12	0.49
1:B:92:ILE:HG23	1:B:97:LEU:HB2	1.95	0.49
1:A:339:THR:O	1:A:340:ASP:HB3	2.13	0.49
1:A:570:LEU:O	1:A:571:GLU:C	2.51	0.49
1:A:546:VAL:HG11	1:A:556:ILE:HG23	1.95	0.49
1:A:126:ASP:O	1:A:128:THR:N	2.46	0.49
1:A:93:ASP:O	1:A:96:LYS:N	2.43	0.49
1:C:320:LYS:CE	1:C:326:GLU:HG2	2.43	0.49
1:A:364:ARG:HA	1:A:367:ARG:HD3	1.95	0.49
1:A:336:LEU:HD22	1:A:352:VAL:CG1	2.42	0.49
1:A:204:ARG:HD3	1:A:378:TYR:CE1	2.47	0.49
1:C:115:ALA:HB1	1:C:161:GLU:O	2.13	0.49
1:A:317:GLU:HA	1:A:320:LYS:HB2	1.95	0.49
1:B:528:GLY:O	1:B:534:ASP:HB2	2.12	0.49
1:C:59:MET:CE	1:C:82:PRO:HA	2.42	0.49
1:A:134:VAL:HG22	1:A:271:ARG:NH1	2.28	0.49
1:C:270:PRO:HB3	1:C:315:ALA:HB2	1.94	0.48
1:C:159:LYS:HE2	1:C:159:LYS:N	2.29	0.48
2:C:576:PPS:N3	2:C:576:PPS:H5'2	2.29	0.48
1:A:115:ALA:HA	1:A:163:VAL:HG12	1.94	0.48
1:A:6:HIS:HB3	1:A:53:SER:O	2.12	0.48
1:B:339:THR:O	1:B:340:ASP:HB3	2.14	0.48
1:A:362:LEU:HD22	1:A:376:PHE:CE2	2.48	0.48
1:A:48:MET:HE2	1:A:162:ALA:HB1	1.95	0.48
1:A:184:HIS:NE2	1:A:188:LEU:HD11	2.28	0.48
1:C:337:PRO:HG2	1:C:355:LEU:HG	1.94	0.48
1:C:425:GLY:HA2	1:C:573:GLN:HE22	1.78	0.48
1:B:330:PHE:HD1	1:B:332:MET:H	1.60	0.48
1:A:449:GLU:HG3	3:A:657:HOH:O	2.13	0.48
1:A:39:ARG:HD2	3:A:626:HOH:O	2.13	0.48
1:C:207:ARG:NE	1:C:250:ARG:O	2.42	0.48
1:A:11:LYS:N	1:A:11:LYS:HD2	2.29	0.48
1:B:59:MET:CE	1:B:83:ILE:H	2.26	0.48
1:B:90:GLU:O	1:B:94:GLU:N	2.43	0.48
1:B:547:ASP:OD1	1:B:549:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:HG3	1:B:275:TRP:HE3	1.77	0.48
1:A:71:ASN:OD1	1:A:80:SER:HB3	2.13	0.48
1:B:507:GLU:H	1:B:507:GLU:CD	2.17	0.48
1:C:339:THR:O	1:C:340:ASP:HB3	2.14	0.48
1:A:336:LEU:O	1:A:340:ASP:N	2.31	0.48
1:A:344:PRO:C	1:A:346:ASP:H	2.16	0.48
1:B:570:LEU:O	1:B:571:GLU:C	2.51	0.48
1:C:534:ASP:OD2	1:C:535:PRO:HD2	2.13	0.48
1:B:423:GLN:HE22	1:B:425:GLY:HA3	1.78	0.48
1:C:527:LYS:HG2	1:C:528:GLY:H	1.79	0.48
1:A:197:GLN:HE22	1:A:226:VAL:HG21	1.79	0.48
1:A:171:TYR:CD1	1:A:241:VAL:HG11	2.48	0.48
1:A:172:VAL:HG22	3:A:622:HOH:O	2.13	0.48
1:A:171:TYR:CE1	1:A:241:VAL:HG11	2.49	0.48
1:B:11:LYS:HD2	1:B:11:LYS:N	2.27	0.48
1:C:202:MET:HA	1:C:206:HIS:ND1	2.28	0.48
1:B:336:LEU:O	1:B:340:ASP:N	2.33	0.48
1:B:21:GLN:HA	3:B:630:HOH:O	2.14	0.48
1:A:392:ARG:HD2	1:A:569:PHE:CZ	2.49	0.48
1:B:115:ALA:HA	1:B:163:VAL:HG13	1.95	0.47
1:B:121:ASP:OD1	1:B:123:TYR:HD2	1.97	0.47
1:C:378:TYR:HB3	1:C:380:GLU:OE1	2.13	0.47
1:B:346:ASP:C	1:B:348:VAL:H	2.18	0.47
1:C:423:GLN:HE21	1:C:425:GLY:N	2.02	0.47
1:B:302:LYS:HE3	1:B:304:GLU:OE2	2.13	0.47
1:C:392:ARG:HD2	1:C:569:PHE:CZ	2.50	0.47
1:C:330:PHE:CD1	1:C:330:PHE:O	2.67	0.47
1:A:114:LEU:C	1:A:163:VAL:HG13	2.33	0.47
1:A:101:SER:HB2	1:A:119:ILE:HD12	1.95	0.47
1:B:378:TYR:HB3	1:B:380:GLU:OE1	2.14	0.47
1:C:364:ARG:HA	1:C:367:ARG:HD3	1.96	0.47
1:C:114:LEU:HD13	1:C:166:LEU:CD2	2.37	0.47
1:C:448:ARG:NH1	1:C:482:GLU:OE1	2.47	0.47
1:C:290:VAL:HG23	1:C:327:VAL:HG13	1.96	0.47
1:B:286:THR:HG1	1:B:287:HIS:HD2	1.59	0.47
1:B:357:ILE:HB	1:B:376:PHE:CE1	2.50	0.47
1:A:432:LEU:HD23	1:A:475:ALA:HB3	1.95	0.47
1:C:80:SER:HB2	1:C:271:ARG:HD3	1.97	0.47
1:A:507:GLU:CD	1:A:507:GLU:H	2.16	0.47
1:C:208:GLU:O	1:C:212:ARG:CG	2.57	0.47
1:C:61:GLN:NE2	1:C:65:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD11	1:A:83:ILE:CG2	2.43	0.47
1:B:263:LEU:HD11	1:B:275:TRP:CH2	2.49	0.47
1:C:290:VAL:CG2	1:C:327:VAL:HG13	2.45	0.47
1:A:488:ARG:O	1:A:492:SER:OG	2.29	0.47
1:C:546:VAL:HG21	1:C:556:ILE:HG23	1.97	0.47
1:C:1:MET:CG	1:C:2:ALA:N	2.78	0.47
1:B:190:TRP:CH2	1:B:257:VAL:HG23	2.50	0.47
1:B:122:ILE:HG22	1:B:122:ILE:O	2.15	0.47
1:A:140:GLU:CD	1:A:301:SER:H	2.18	0.46
1:C:360:THR:O	1:C:364:ARG:HB2	2.15	0.46
1:C:414:ARG:NH2	3:C:754:HOH:O	2.39	0.46
1:B:448:ARG:NH1	1:B:482:GLU:OE1	2.47	0.46
1:B:127:LYS:HD3	1:B:147:LEU:O	2.14	0.46
1:B:361:GLU:O	1:B:365:ARG:HG3	2.15	0.46
1:C:546:VAL:HG11	1:C:556:ILE:HG23	1.97	0.46
1:A:388:SER:CB	3:A:642:HOH:O	2.63	0.46
1:B:274:ILE:HD11	1:B:315:ALA:HB1	1.96	0.46
1:B:519:ALA:HB3	3:B:674:HOH:O	2.15	0.46
1:C:206:HIS:O	1:C:209:LEU:HB3	2.15	0.46
1:B:339:THR:HG22	1:B:341:GLU:CD	2.36	0.46
1:B:48:MET:HG2	1:B:162:ALA:HB2	1.96	0.46
1:B:364:ARG:HA	1:B:367:ARG:HD3	1.96	0.46
1:C:203:HIS:HE1	1:C:385:LEU:CD1	2.29	0.46
1:A:199:ARG:NH1	1:A:265:MET:CE	2.78	0.46
1:A:171:TYR:HB3	1:A:174:LEU:HD12	1.97	0.46
1:B:452:HIS:O	1:B:456:GLN:HG3	2.16	0.46
1:A:346:ASP:C	1:A:348:VAL:H	2.19	0.46
1:A:40:GLN:NE2	1:A:85:LEU:HD12	2.30	0.46
1:A:378:TYR:HB3	1:A:380:GLU:OE1	2.16	0.46
1:A:5:PRO:O	1:A:281:LYS:HE3	2.16	0.46
1:B:40:GLN:NE2	1:B:85:LEU:HD12	2.30	0.46
1:A:208:GLU:HA	1:A:208:GLU:OE2	2.15	0.46
1:B:316:VAL:O	1:B:320:LYS:HB2	2.15	0.46
1:A:1:MET:SD	1:A:4:ALA:HA	2.56	0.46
1:A:225:PRO:HD2	1:A:259:GLY:O	2.15	0.46
1:C:362:LEU:HD22	1:C:376:PHE:CE2	2.50	0.46
1:C:266:ARG:O	1:C:267:MET:HB2	2.16	0.46
1:A:217:ARG:HG2	1:A:217:ARG:HH11	1.81	0.46
1:C:346:ASP:C	1:C:348:VAL:H	2.18	0.46
1:B:546:VAL:HG11	1:B:556:ILE:HG21	1.96	0.46
1:A:372:ILE:HA	1:A:373:PRO:HD3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:TYR:HB2	1:C:181:LEU:HD22	1.99	0.45
1:C:216:SER:C	1:C:218:GLN:H	2.18	0.45
1:C:339:THR:HG22	1:C:341:GLU:CD	2.37	0.45
1:A:24:LEU:HD23	1:A:116:ILE:HD12	1.98	0.45
1:C:263:LEU:HD11	1:C:275:TRP:CH2	2.51	0.45
1:A:113:ASN:O	1:A:164:ASN:HB2	2.17	0.45
1:C:312:ALA:HB3	3:C:620:HOH:O	2.16	0.45
1:C:333:VAL:HG23	1:C:342:TYR:HB3	1.99	0.45
1:A:119:ILE:CG2	1:A:120:ASP:N	2.79	0.45
1:A:109:ARG:NE	1:A:229:LEU:HD13	2.31	0.45
1:A:357:ILE:HB	1:A:376:PHE:CE1	2.51	0.45
1:B:392:ARG:HD2	1:B:569:PHE:CZ	2.52	0.45
1:A:292:ARG:CZ	1:A:292:ARG:HB3	2.46	0.45
1:A:98:GLN:HA	1:A:122:ILE:HD12	1.98	0.45
1:C:231:LYS:HB2	1:C:234:ASP:CB	2.46	0.45
1:B:88:SER:O	1:B:92:ILE:HG13	2.17	0.45
1:A:72:ARG:NH1	1:A:76:GLY:O	2.48	0.45
1:C:344:PRO:C	1:C:346:ASP:H	2.20	0.45
1:A:349:PRO:O	1:A:352:VAL:HG23	2.17	0.45
1:C:546:VAL:CG1	1:C:556:ILE:CD1	2.94	0.45
1:B:441:SER:OG	1:B:454:ASN:ND2	2.48	0.45
1:C:349:PRO:O	1:C:352:VAL:HG23	2.16	0.45
1:B:344:PRO:C	1:B:346:ASP:H	2.20	0.45
1:A:36:LEU:HD21	1:A:105:LEU:HD22	1.98	0.45
1:A:313:GLN:HB3	1:A:329:GLU:CG	2.43	0.45
1:C:197:GLN:HE22	1:C:265:MET:HE2	1.80	0.45
1:A:270:PRO:HG3	1:A:311:ASP:C	2.37	0.45
1:A:66:ARG:O	1:A:70:ASP:HB2	2.16	0.45
1:A:330:PHE:CD1	1:A:330:PHE:O	2.69	0.45
1:A:73:LEU:HG	1:A:79:PHE:HB3	1.99	0.45
1:C:357:ILE:HB	1:C:376:PHE:CE1	2.52	0.45
1:A:240:ARG:NH1	1:A:244:TYR:OH	2.50	0.45
1:A:291:GLY:CA	1:A:330:PHE:CE2	3.00	0.45
1:C:203:HIS:N	1:C:206:HIS:ND1	2.47	0.44
1:B:362:LEU:HD22	1:B:376:PHE:CE2	2.52	0.44
1:B:330:PHE:O	1:B:330:PHE:CD1	2.70	0.44
1:B:477:ILE:CG2	1:B:479:PRO:HG3	2.46	0.44
1:C:204:ARG:HH11	1:C:204:ARG:HG2	1.83	0.44
1:C:250:ARG:HH21	1:C:379:PRO:HD2	1.82	0.44
1:A:88:SER:O	1:A:92:ILE:HG13	2.16	0.44
1:C:392:ARG:NH1	1:C:567:GLN:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:O	1:A:130:GLU:C	2.55	0.44
1:C:214:ALA:HB3	1:C:255:MET:CE	2.47	0.44
1:A:423:GLN:NE2	1:A:425:GLY:HA3	2.32	0.44
1:A:36:LEU:HD22	1:A:85:LEU:HD13	1.99	0.44
1:A:447:THR:O	1:A:448:ARG:C	2.55	0.44
1:A:109:ARG:HD3	1:A:229:LEU:HD13	1.99	0.44
1:A:95:LYS:O	1:A:96:LYS:HB2	2.18	0.44
1:A:98:GLN:O	1:A:99:ALA:C	2.56	0.44
1:C:411:ALA:HA	3:C:750:HOH:O	2.17	0.44
1:A:204:ARG:HD2	1:A:204:ARG:O	2.17	0.44
1:C:255:MET:HG2	1:C:255:MET:O	2.17	0.44
1:C:90:GLU:CD	1:C:90:GLU:H	2.21	0.44
1:B:443:GLU:HB2	3:B:654:HOH:O	2.16	0.44
1:A:337:PRO:HG3	1:A:355:LEU:CD1	2.47	0.44
1:A:423:GLN:NE2	1:A:425:GLY:CA	2.81	0.44
1:A:434:ASP:HB3	2:A:574:PPS:O3P	2.18	0.44
1:B:108:PHE:C	1:B:108:PHE:CD1	2.91	0.44
1:A:133:LEU:HD23	1:A:133:LEU:N	2.33	0.44
1:C:197:GLN:HE22	1:C:265:MET:CE	2.31	0.44
1:A:141:HIS:HA	1:A:142:PRO:HD3	1.86	0.44
1:B:90:GLU:CD	1:B:90:GLU:H	2.20	0.44
1:C:546:VAL:HG11	1:C:556:ILE:HG21	2.00	0.44
1:A:226:VAL:HG12	1:A:227:VAL:N	2.33	0.44
1:A:190:TRP:CH2	1:A:257:VAL:HG23	2.52	0.44
1:C:510:GLU:HG2	1:C:518:TYR:CG	2.53	0.44
1:C:190:TRP:CZ3	1:C:257:VAL:HG23	2.52	0.44
1:C:48:MET:HE1	1:C:164:ASN:O	2.17	0.44
1:B:437:ARG:HA	1:B:437:ARG:HD2	1.87	0.44
1:A:339:THR:HG22	1:A:341:GLU:CD	2.38	0.43
1:B:48:MET:HE2	1:B:114:LEU:O	2.19	0.43
1:C:217:ARG:HG2	1:C:217:ARG:NH1	2.31	0.43
1:A:448:ARG:NH1	1:A:482:GLU:OE1	2.50	0.43
1:C:510:GLU:HG2	1:C:518:TYR:CD2	2.53	0.43
1:A:333:VAL:HG23	1:A:342:TYR:HB3	2.00	0.43
1:A:31:LEU:HD22	1:A:102:ARG:O	2.17	0.43
1:B:451:ARG:HH12	2:B:575:PPS:C2	2.31	0.43
1:C:204:ARG:NH2	1:C:342:TYR:OH	2.50	0.43
1:A:528:GLY:O	1:A:534:ASP:HB2	2.19	0.43
1:A:292:ARG:HH21	1:A:309:PRO:HB3	1.82	0.43
1:A:26:ALA:O	1:A:29:GLU:HB2	2.18	0.43
1:C:296:GLY:HA2	1:C:297:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ALA:HB1	1:A:525:GLU:HB2	2.00	0.43
1:B:81:MET:SD	1:B:82:PRO:HD2	2.58	0.43
1:A:176:TYR:CB	1:A:181:LEU:HD13	2.48	0.43
1:A:314:HIS:O	1:A:317:GLU:HG2	2.18	0.43
1:C:390:PRO:HA	1:C:391:PRO:HD3	1.80	0.43
1:B:250:ARG:HA	1:B:250:ARG:HD3	1.72	0.43
1:C:138:ASP:HA	1:C:139:PRO:HD3	1.79	0.43
1:B:44:LEU:HA	1:B:47:ILE:HD12	2.01	0.43
1:A:452:HIS:O	1:A:456:GLN:HG3	2.18	0.43
1:A:274:ILE:HD11	1:A:315:ALA:O	2.19	0.43
1:B:98:GLN:O	1:B:99:ALA:C	2.55	0.43
1:A:337:PRO:HG2	1:A:355:LEU:HG	2.00	0.43
1:B:214:ALA:HB2	1:B:221:VAL:CG2	2.49	0.43
1:B:202:MET:HA	1:B:206:HIS:ND1	2.33	0.43
1:A:572:ARG:HD2	1:B:253:ASN:OD1	2.19	0.43
1:A:126:ASP:C	1:A:128:THR:H	2.22	0.43
1:C:334:THR:OG1	1:C:335:TYR:N	2.52	0.43
1:A:16:ARG:O	1:A:18:ALA:N	2.51	0.43
1:C:207:ARG:HD3	1:C:207:ARG:C	2.39	0.43
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.79	0.43
1:A:192:ARG:HG3	1:A:219:ALA:HA	2.00	0.43
1:B:138:ASP:HA	1:B:139:PRO:HD3	1.88	0.43
1:A:193:VAL:H	1:A:286:THR:CG2	2.29	0.43
1:A:425:GLY:HA2	1:A:573:GLN:HE22	1.84	0.43
1:A:1:MET:CE	1:A:5:PRO:HD3	2.49	0.43
1:A:390:PRO:HA	1:A:391:PRO:HD3	1.80	0.43
1:B:349:PRO:O	1:B:352:VAL:HG23	2.19	0.42
1:C:36:LEU:HB3	1:C:40:GLN:HB2	2.00	0.42
1:A:71:ASN:OD1	1:A:80:SER:CB	2.67	0.42
1:C:544:LEU:HD11	1:C:559:GLU:OE2	2.19	0.42
1:B:103:ILE:O	1:B:116:ILE:HA	2.19	0.42
1:C:202:MET:HB3	1:C:247:LEU:HD22	2.01	0.42
1:C:208:GLU:O	1:C:209:LEU:C	2.56	0.42
1:A:302:LYS:HG3	1:A:304:GLU:OE2	2.19	0.42
1:A:546:VAL:CG1	1:A:556:ILE:CD1	2.97	0.42
1:A:74:ALA:O	1:A:76:GLY:N	2.50	0.42
1:C:512:SER:O	1:C:514:LYS:HG3	2.18	0.42
1:C:212:ARG:NH2	1:C:342:TYR:HD1	2.17	0.42
1:A:119:ILE:HG22	1:A:121:ASP:N	2.34	0.42
1:B:272:GLU:HG2	1:B:276:HIS:CD2	2.54	0.42
1:B:432:LEU:HD23	1:B:432:LEU:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PRO:CD	1:B:353:LYS:CB	2.89	0.42
1:A:572:ARG:HD2	1:B:253:ASN:CB	2.48	0.42
1:A:39:ARG:NH1	1:A:266:ARG:HG3	2.34	0.42
1:C:1:MET:HG3	1:C:2:ALA:H	1.83	0.42
1:B:512:SER:O	1:B:514:LYS:HG3	2.20	0.42
1:A:89:GLN:HA	1:A:92:ILE:HD12	2.02	0.42
1:A:59:MET:HE3	1:A:67:VAL:HG21	1.99	0.42
1:C:102:ARG:NH2	1:C:161:GLU:OE1	2.52	0.42
1:A:273:ALA:O	1:A:276:HIS:HB2	2.20	0.42
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.76	0.42
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.65	0.42
1:B:562:LEU:HA	1:B:562:LEU:HD23	1.78	0.42
1:C:204:ARG:H	1:C:377:SER:HA	1.84	0.42
1:B:192:ARG:HD2	1:B:217:ARG:O	2.20	0.42
1:B:272:GLU:O	1:B:275:TRP:HB3	2.19	0.42
1:B:192:ARG:HB3	1:B:219:ALA:HB2	2.02	0.42
1:C:36:LEU:HB2	1:C:41:LEU:HG	2.02	0.42
1:B:299:SER:HA	1:B:304:GLU:O	2.19	0.42
1:B:117:LEU:C	1:B:117:LEU:CD2	2.86	0.42
1:B:250:ARG:HG3	1:B:378:TYR:CD2	2.55	0.42
1:B:451:ARG:HH12	2:B:575:PPS:H2	1.85	0.42
1:A:292:ARG:O	1:A:293:ASP:HB2	2.19	0.42
1:B:333:VAL:HG23	1:B:342:TYR:HB3	2.01	0.42
1:C:27:GLU:HG2	1:C:31:LEU:HD11	2.02	0.42
1:C:299:SER:HB3	1:C:305:ASP:OD1	2.20	0.42
1:A:251:TYR:O	1:A:252:PRO:C	2.57	0.42
1:A:138:ASP:HA	1:A:139:PRO:HD3	1.78	0.42
1:A:140:GLU:O	1:A:145:VAL:HG23	2.19	0.41
1:A:197:GLN:HG2	1:A:294:HIS:CE1	2.54	0.41
1:A:138:ASP:OD2	1:A:138:ASP:C	2.59	0.41
1:C:57:GLY:HA2	1:C:160:ILE:HG13	2.01	0.41
1:B:546:VAL:HG21	1:B:556:ILE:HG23	2.02	0.41
1:C:89:GLN:HB3	1:C:90:GLU:OE1	2.19	0.41
1:C:440:LEU:O	1:C:457:ARG:NH1	2.40	0.41
1:C:507:GLU:H	1:C:507:GLU:CD	2.24	0.41
1:A:565:GLU:CB	3:A:655:HOH:O	2.68	0.41
1:A:223:ILE:HD11	1:A:251:TYR:CE1	2.55	0.41
1:C:98:GLN:HA	1:C:122:ILE:CD1	2.51	0.41
1:A:477:ILE:CG2	1:A:479:PRO:HG3	2.50	0.41
1:C:98:GLN:O	1:C:99:ALA:C	2.57	0.41
1:B:20:ARG:HD2	3:B:622:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PRO:HG3	1:B:355:LEU:CD1	2.49	0.41
1:A:36:LEU:HD11	1:A:105:LEU:HB3	2.03	0.41
1:A:477:ILE:HG22	1:A:479:PRO:HG3	2.02	0.41
1:A:334:THR:OG1	1:A:335:TYR:N	2.53	0.41
1:B:48:MET:HE2	1:B:115:ALA:HB2	1.94	0.41
1:B:217:ARG:HH11	1:B:217:ARG:HG2	1.85	0.41
1:A:362:LEU:HD22	1:A:376:PHE:HE2	1.85	0.41
1:C:345:VAL:HG11	3:C:693:HOH:O	2.17	0.41
1:B:501:HIS:CE1	1:B:539:PRO:HD2	2.55	0.41
1:C:47:ILE:HG13	1:C:52:PHE:HD1	1.86	0.41
1:C:337:PRO:HG3	1:C:355:LEU:CD1	2.47	0.41
1:A:109:ARG:HH21	1:A:166:LEU:CD1	2.34	0.41
1:A:31:LEU:CD2	1:A:102:ARG:HB3	2.45	0.41
1:C:92:ILE:HA	1:C:97:LEU:HD12	2.02	0.41
1:B:313:GLN:NE2	1:B:329:GLU:HG2	2.35	0.41
1:A:117:LEU:C	1:A:117:LEU:HD23	2.41	0.41
1:A:510:GLU:HG2	1:A:518:TYR:CD2	2.56	0.41
1:C:203:HIS:NE2	1:C:362:LEU:HD21	2.36	0.41
1:C:423:GLN:NE2	1:C:425:GLY:HA3	2.36	0.41
1:A:153:GLU:HG2	1:A:154:PHE:CD2	2.55	0.41
1:B:392:ARG:NH1	1:B:567:GLN:O	2.52	0.41
1:A:90:GLU:O	1:A:94:GLU:CB	2.64	0.41
1:A:117:LEU:HA	1:A:160:ILE:HD13	2.02	0.41
1:B:447:THR:O	1:B:448:ARG:C	2.59	0.41
1:C:436:VAL:HG11	1:C:458:ILE:HD11	2.02	0.41
1:A:440:LEU:O	1:A:457:ARG:HD3	2.21	0.41
1:C:547:ASP:OD1	1:C:549:SER:HB2	2.21	0.41
1:B:131:ALA:HB1	1:B:144:ILE:CD1	2.50	0.41
1:C:18:ALA:O	1:C:21:GLN:HB2	2.20	0.41
1:C:245:GLN:O	1:C:248:LEU:HB2	2.21	0.41
1:B:86:ASP:HA	1:B:154:PHE:O	2.21	0.41
1:A:103:ILE:O	1:A:116:ILE:HA	2.21	0.40
1:A:129:LYS:CE	1:A:133:LEU:HD11	2.48	0.40
1:A:552:SER:O	1:A:556:ILE:HG13	2.21	0.40
2:B:575:PPS:H5'2	2:B:575:PPS:N3	2.35	0.40
1:C:504:THR:HA	1:C:505:PRO:HD3	1.96	0.40
1:C:246:ALA:O	1:C:249:PRO:HD2	2.21	0.40
1:C:46:LEU:O	1:C:51:GLY:N	2.54	0.40
1:A:296:GLY:HA2	1:A:297:PRO:HD3	1.88	0.40
1:C:250:ARG:HG3	1:C:378:TYR:CD2	2.56	0.40
1:B:209:LEU:HD13	1:B:330:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ILE:HA	1:C:373:PRO:HD3	1.84	0.40
1:C:41:LEU:HD22	1:C:166:LEU:HD13	2.02	0.40
1:A:32:PRO:HB3	1:A:95:LYS:HB3	2.03	0.40
1:B:93:ASP:O	1:B:94:GLU:C	2.59	0.40
1:A:200:ASN:HB3	1:A:201:PRO:CD	2.51	0.40
1:B:92:ILE:HD13	1:B:122:ILE:HG21	2.04	0.40
1:C:269:GLY:HA3	1:C:270:PRO:HD3	1.91	0.40
1:C:447:THR:O	1:C:448:ARG:C	2.59	0.40
1:C:374:GLU:HG3	1:C:379:PRO:HD3	2.04	0.40
1:A:109:ARG:CD	1:A:229:LEU:HD13	2.51	0.40
1:B:312:ALA:HB3	3:B:584:HOH:O	2.21	0.40
1:B:370:ALA:O	1:B:371:HIS:C	2.60	0.40
1:C:292:ARG:HA	1:C:309:PRO:O	2.21	0.40
1:A:512:SER:O	1:A:514:LYS:HG3	2.21	0.40
1:C:333:VAL:HB	1:C:343:ARG:O	2.21	0.40
1:C:528:GLY:O	1:C:534:ASP:HB2	2.22	0.40
1:C:546:VAL:HG11	1:C:556:ILE:CD1	2.51	0.40
1:C:249:PRO:C	1:C:251:TYR:H	2.25	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	571/573 (100%)	492 (86%)	56 (10%)	23 (4%)	4	4
1	B	571/573 (100%)	513 (90%)	47 (8%)	11 (2%)	10	19
1	C	571/573 (100%)	517 (90%)	46 (8%)	8 (1%)	14	28
All	All	1713/1719 (100%)	1522 (89%)	149 (9%)	42 (2%)	7	12

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	75	ASP
1	A	571	GLU
1	B	571	GLU
1	C	571	GLU
1	A	2	ALA
1	A	16	ARG
1	A	94	GLU
1	A	127	LYS
1	A	138	ASP
1	A	166	LEU
1	A	202	MET
1	A	352	VAL
1	A	572	ARG
1	B	94	GLU
1	B	352	VAL
1	B	371	HIS
1	C	352	VAL
1	C	371	HIS
1	C	572	ARG
1	A	131	ALA
1	A	232	PRO
1	A	269	GLY
1	A	371	HIS
1	A	528	GLY
1	B	202	MET
1	B	528	GLY
1	B	572	ARG
1	A	5	PRO
1	A	99	ALA
1	A	130	GLU
1	A	141	HIS
1	C	424	GLY
1	C	528	GLY
1	B	347	GLN
1	B	503	ALA
1	C	503	ALA
1	B	269	GLY
1	B	344	PRO
1	C	344	PRO
1	A	122	ILE
1	A	344	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	472/474 (100%)	438 (93%)	34 (7%)	18	35
1	B	472/474 (100%)	448 (95%)	24 (5%)	29	55
1	C	472/474 (100%)	452 (96%)	20 (4%)	36	65
All	All	1416/1422 (100%)	1338 (94%)	78 (6%)	27	51

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ASN
1	A	11	LYS
1	A	23	GLU
1	A	24	LEU
1	A	41	LEU
1	A	66	ARG
1	A	70	ASP
1	A	133	LEU
1	A	144	ILE
1	A	154	PHE
1	A	163	VAL
1	A	166	LEU
1	A	191	SER
1	A	192	ARG
1	A	199	ARG
1	A	224	HIS
1	A	225	PRO
1	A	239	THR
1	A	240	ARG
1	A	248	LEU
1	A	280	ARG
1	A	302	LYS
1	A	338	ASP
1	A	339	THR
1	A	342	TYR

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Mol	Chain	Res	Type
1	A	355	LEU
1	A	361	GLU
1	A	364	ARG
1	A	423	GLN
1	A	426	ARG
1	A	437	ARG
1	A	448	ARG
1	A	573	GLN
1	B	3	ASN
1	B	11	LYS
1	B	14	LEU
1	B	21	GLN
1	B	90	GLU
1	B	94	GLU
1	B	181	LEU
1	B	192	ARG
1	B	199	ARG
1	B	209	LEU
1	B	240	ARG
1	B	248	LEU
1	B	338	ASP
1	B	339	THR
1	B	342	TYR
1	B	355	LEU
1	B	361	GLU
1	B	364	ARG
1	B	410	ASP
1	B	423	GLN
1	B	426	ARG
1	B	437	ARG
1	B	448	ARG
1	B	573	GLN
1	C	3	ASN
1	C	19	PRO
1	C	70	ASP
1	C	90	GLU
1	C	159	LYS
1	C	166	LEU
1	C	181	LEU
1	C	199	ARG
1	C	240	ARG
1	C	248	LEU

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Mol	Chain	Res	Type
1	C	338	ASP
1	C	342	TYR
1	C	355	LEU
1	C	361	GLU
1	C	364	ARG
1	C	423	GLN
1	C	426	ARG
1	C	437	ARG
1	C	448	ARG
1	C	573	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	167	ASN
1	A	331	GLN
1	A	423	GLN
1	A	454	ASN
1	A	456	GLN
1	A	573	GLN
1	B	3	ASN
1	B	77	ASN
1	B	167	ASN
1	B	287	HIS
1	B	331	GLN
1	B	423	GLN
1	B	454	ASN
1	B	456	GLN
1	B	573	GLN
1	C	3	ASN
1	C	89	GLN
1	C	167	ASN
1	C	287	HIS
1	C	331	GLN
1	C	423	GLN
1	C	454	ASN
1	C	456	GLN
1	C	573	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PPS	A	574	-	26,33,33	1.56	3 (11%)	31,52,52	1.44	4 (12%)
2	PPS	B	575	-	26,33,33	1.70	5 (19%)	31,52,52	1.49	5 (16%)
2	PPS	C	576	-	26,33,33	1.74	3 (11%)	31,52,52	1.51	5 (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
2	PPS	A	574	-	-	0/11/37/37	0/3/3/3
2	PPS	B	575	-	-	0/11/37/37	0/3/3/3
2	PPS	C	576	-	-	0/11/37/37	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	576	PPS	C8-N7	-2.40	1.30	1.34
2	B	575	PPS	C8-N7	-2.12	1.30	1.34
2	B	575	PPS	O5'-C5'	-2.04	1.36	1.44
2	A	574	PPS	C2-N1	2.24	1.38	1.33
2	A	574	PPS	C4-N3	2.33	1.39	1.35
2	B	575	PPS	C2-N1	2.48	1.38	1.33
2	C	576	PPS	C2-N1	2.79	1.39	1.33
2	B	575	PPS	C4-N3	2.81	1.39	1.35
2	A	574	PPS	O4'-C1'	5.27	1.47	1.41
2	B	575	PPS	O4'-C1'	5.34	1.48	1.41
2	C	576	PPS	O4'-C1'	6.35	1.49	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	574	PPS	C2'-C3'-C4'	-2.77	98.08	103.29
2	B	575	PPS	C2'-C3'-C4'	-2.47	98.65	103.29
2	C	576	PPS	O3'-C3'-C2'	-2.15	103.16	111.51
2	A	574	PPS	C1'-N9-C4	2.20	130.25	126.94
2	B	575	PPS	O6P-P2-O5'	2.32	109.11	102.97
2	C	576	PPS	C1'-N9-C4	2.41	130.57	126.94
2	B	575	PPS	O2P-P1-O1P	2.48	116.82	107.38
2	B	575	PPS	C1'-N9-C4	2.50	130.72	126.94
2	A	574	PPS	O2P-P1-O1P	2.70	117.67	107.38
2	B	575	PPS	N3-C2-N1	2.78	131.02	128.89
2	C	576	PPS	O2P-P1-O1P	2.79	118.00	107.38
2	C	576	PPS	O4'-C1'-N9	2.89	114.15	108.10
2	A	574	PPS	N3-C2-N1	3.17	131.32	128.89
2	C	576	PPS	N3-C2-N1	3.25	131.39	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	574	PPS	2	0
2	B	575	PPS	4	0
2	C	576	PPS	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	573/573 (100%)	0.25	44 (7%) 16 11	30, 75, 129, 165	0
1	B	573/573 (100%)	-0.03	21 (3%) 45 37	30, 59, 102, 157	0
1	C	573/573 (100%)	-0.07	25 (4%) 38 30	29, 53, 122, 168	0
All	All	1719/1719 (100%)	0.05	90 (5%) 31 24	29, 60, 119, 168	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	GLU	9.3
1	C	350	ALA	7.9
1	B	349	PRO	7.2
1	C	348	VAL	7.2
1	C	1	MET	6.5
1	A	573	GLN	6.3
1	A	348	VAL	5.9
1	B	333	VAL	5.7
1	A	154	PHE	5.6
1	B	527	LYS	5.6
1	C	333	VAL	5.5
1	A	572	ARG	5.5
1	C	349	PRO	5.0
1	A	352	VAL	5.0
1	A	334	THR	5.0
1	A	1	MET	4.8
1	C	352	VAL	4.8
1	A	350	ALA	4.8
1	A	353	LYS	4.6
1	C	334	THR	4.4
1	C	339	THR	4.2
1	C	360	THR	4.2
1	A	349	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	573	GLN	4.0
1	A	360	THR	4.0
1	A	341	GLU	4.0
1	C	343	ARG	4.0
1	B	352	VAL	3.9
1	A	303	GLY	3.9
1	A	354	THR	3.9
1	A	345	VAL	3.7
1	A	305	ASP	3.7
1	C	340	ASP	3.5
1	A	332	MET	3.5
1	C	346	ASP	3.4
1	C	573	GLN	3.4
1	A	91	VAL	3.4
1	A	84	THR	3.2
1	C	372	ILE	3.2
1	A	364	ARG	3.1
1	A	339	THR	3.1
1	B	572	ARG	3.1
1	A	309	PRO	3.1
1	A	300	ASN	3.1
1	A	304	GLU	3.0
1	A	299	SER	3.0
1	B	347	GLN	3.0
1	B	523	ARG	3.0
1	B	348	VAL	3.0
1	A	82	PRO	2.9
1	C	347	GLN	2.8
1	B	343	ARG	2.8
1	A	333	VAL	2.8
1	C	572	ARG	2.8
1	C	2	ALA	2.8
1	A	310	TYR	2.8
1	A	70	ASP	2.8
1	B	334	THR	2.7
1	A	133	LEU	2.7
1	A	306	PHE	2.6
1	B	1	MET	2.6
1	B	350	ALA	2.6
1	A	139	PRO	2.6
1	B	540	GLU	2.5
1	C	353	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	366	LEU	2.5
1	C	382	VAL	2.5
1	C	351	GLY	2.5
1	C	335	TYR	2.4
1	A	346	ASP	2.4
1	B	43	ASP	2.4
1	B	528	GLY	2.4
1	C	370	ALA	2.4
1	A	150	THR	2.4
1	A	311	ASP	2.4
1	C	344	PRO	2.4
1	A	527	LYS	2.3
1	A	298	GLY	2.2
1	A	98	GLN	2.2
1	A	264	ALA	2.2
1	B	344	PRO	2.2
1	C	355	LEU	2.1
1	A	302	LYS	2.1
1	A	47	ILE	2.1
1	B	346	ASP	2.1
1	B	522	ARG	2.1
1	A	137	GLY	2.1
1	A	337	PRO	2.0
1	A	335	TYR	2.0
1	B	353	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	PPS	B	575	31/31	0.95	0.14	-0.72	50,68,96,97	0
2	PPS	A	574	31/31	0.95	0.13	-1.05	59,72,103,111	0
2	PPS	C	576	31/31	0.97	0.11	-1.27	41,59,89,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.