Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:28 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

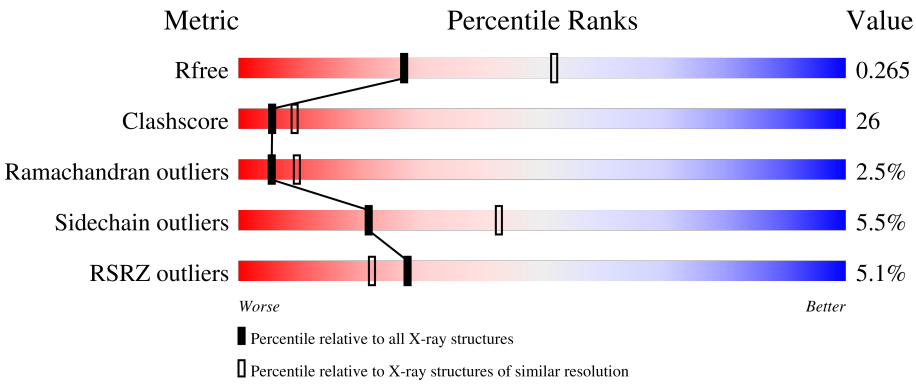
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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	573	8% 51% 42% 7%
1	B	573	3% 64% 31% 5%
1	C	573	4% 63% 33% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14054 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.

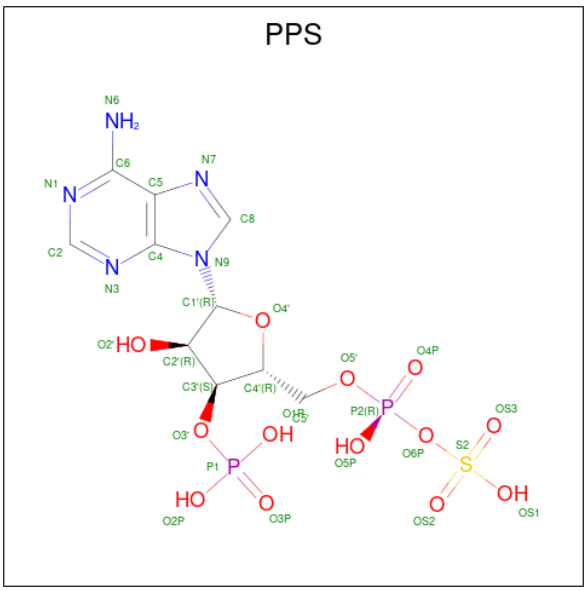
- Molecule 1 is a protein called sulfate adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	573	4501	2832	815	841	13	0	0	0
1	B	573	4501	2832	815	841	13	0	0	0
1	C	573	4501	2832	815	841	13	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	GLY	-	SEE REMARK 999	UNP Q12650
B	369	GLY	-	SEE REMARK 999	UNP Q12650
C	369	GLY	-	SEE REMARK 999	UNP Q12650

- Molecule 2 is 3'-PHOSPHATE-ADENOSINE-5'-PHOSPHATE SULFATE (three-letter code: PPS) (formula: $C_{10}H_{15}N_5O_{13}P_2S$).



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

- Molecule 3 is water.

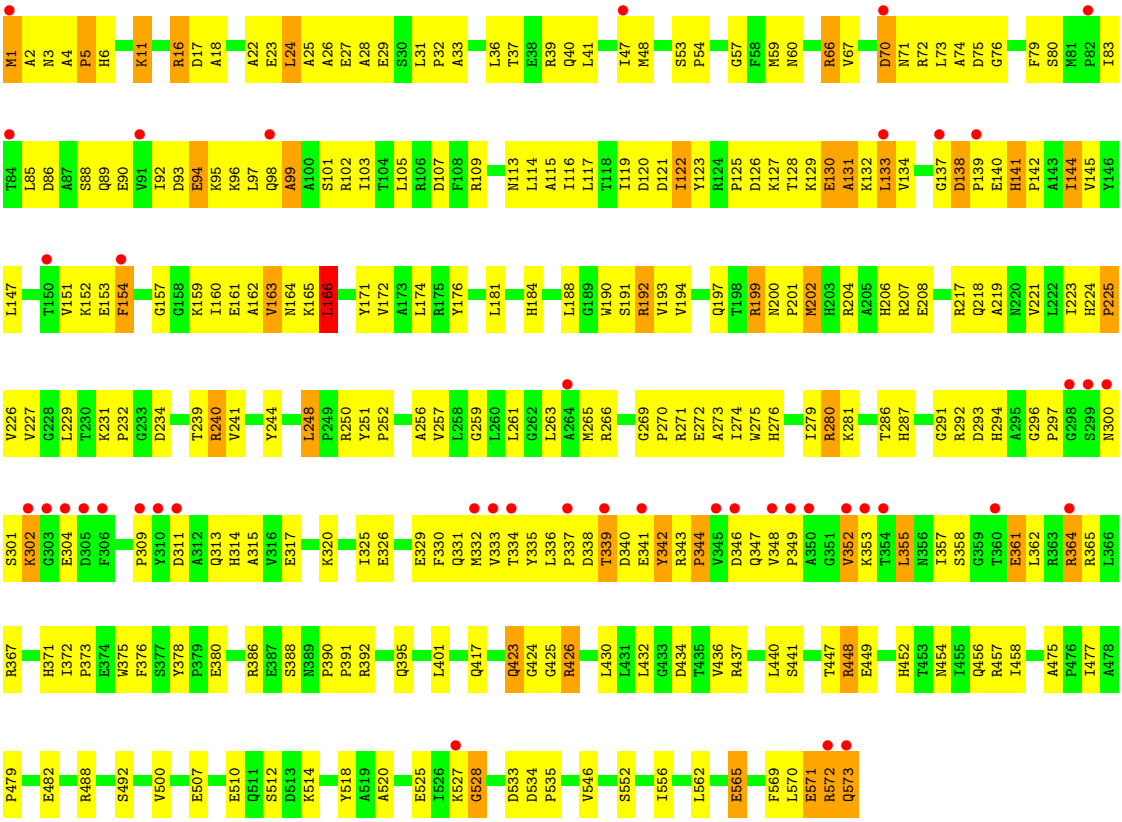
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	100	100	100	0	0
3	B	162	162	162	0	0
3	C	196	196	196	0	0

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.

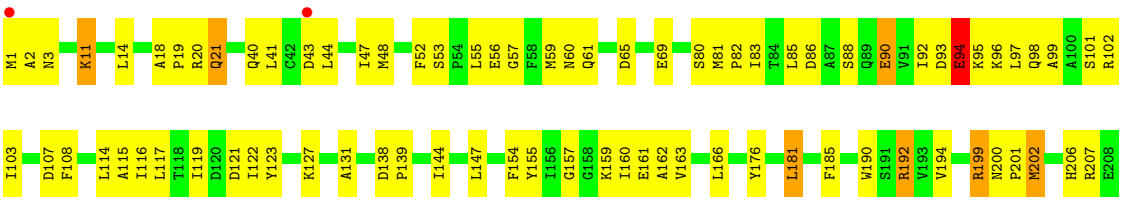
- Molecule 1: sulfate adenylyltransferase

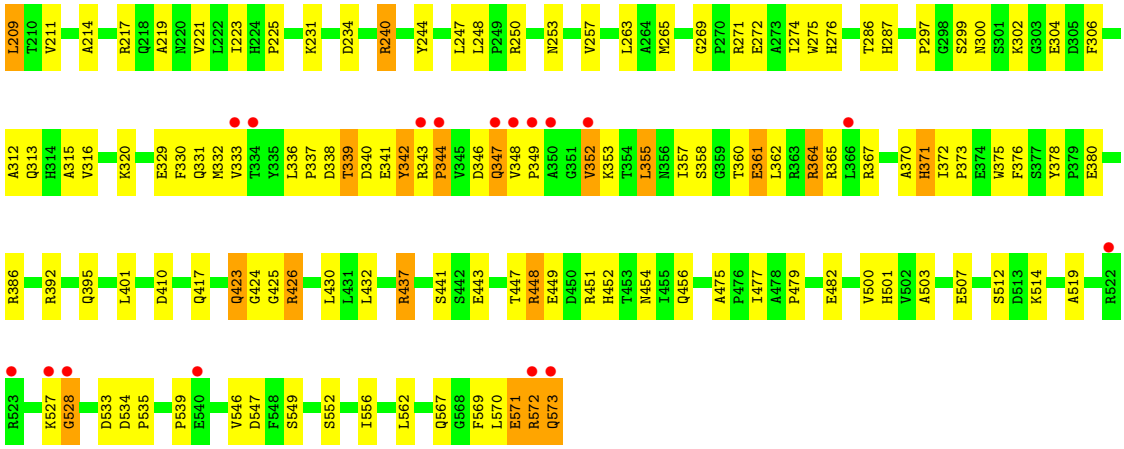
Chain A:



- Molecule 1: sulfate adenylyltransferase

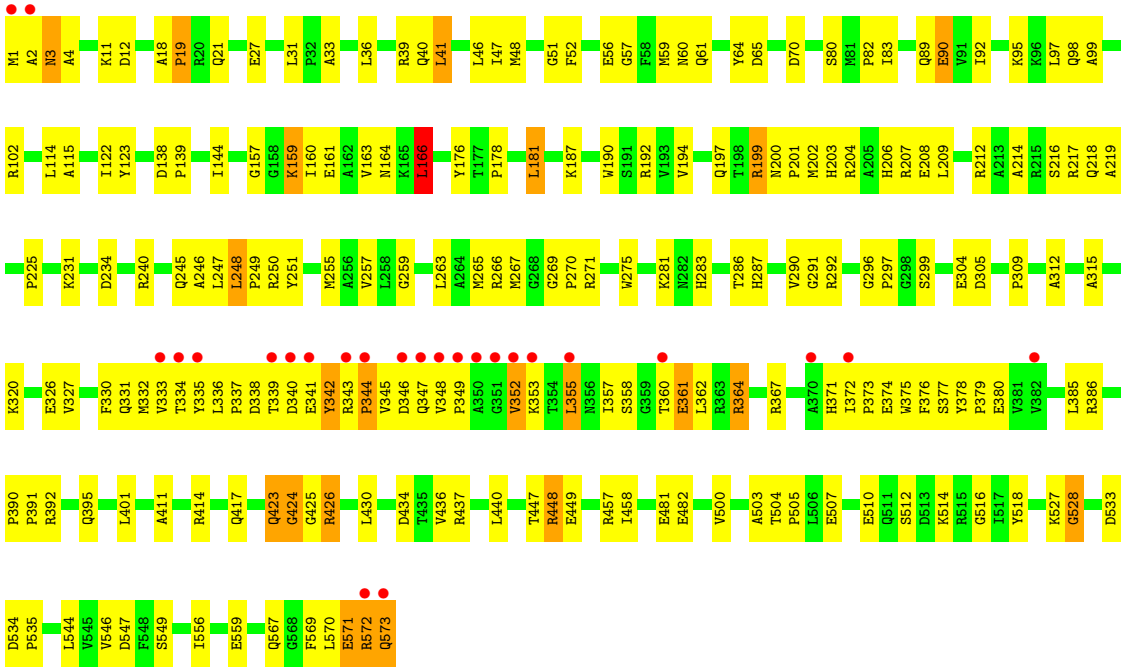
Chain B:





- Molecule 1: sulfate adenylyltransferase

Chain C:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.50 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.272 0.212 , 0.265	Depositor DCC
R_{free} test set	3968 reflections (4.61%)	wwPDB-VP
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 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l	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.*

[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 (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(^{o})	Ideal(^{o})
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:B:423:GLN:HE21	1:B:425:GLY:H	1.08	0.99
1:C:481:GLU:HG3	3:C:647:HOH:O	1.61	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:A:358:SER:HB3	1:A:361:GLU:HB2	1.50	0.94
1:B:358:SER:HB3	1:B: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:HH11	1:B:192:ARG:HB2	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:B:300:ASN:ND2	1:B:304:GLU:HB2	2.04	0.72
1:C:336:LEU:HD22	1:C:352:VAL:HG11	1.70	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:A:60:ASN:HA	1:A:157:GLY:HA3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:PRO:HB2	1:B:347:GLN:HG2	1.73	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:247:LEU:O	1:B:247:LEU:HD12	1.92	0.69
1:B:331:GLN:HE21	1:B:344:PRO:HB3	1.56	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:A:28:ALA:HA	1:A:31:LEU:HD12	1.74	0.69
1:A:202:MET:HA	1:A:206:HIS:ND1	2.08	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:B:59:MET:CE	1:B:82:PRO:HA	2.23	0.69
1:C:357:ILE:HD11	1:C:373:PRO:HG2	1.74	0.69
1:C:3:ASN:HA	3:C:634:HOH:O	1.92	0.68
1:A:59:MET:CE	1:A:67:VAL:HG21	2.24	0.68
1:A:102:ARG:HH11	1:A:116:ILE:HG21	1.58	0.68
1:C:401:LEU:CD2	1:C:500:VAL:HB	2.22	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:A:129:LYS:HE2	1:A:133:LEU:HD11	1.76	0.67
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: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:C:204:ARG:CZ	1:C:342:TYR:OH	2.42	0.67
1:A:313:GLN:HB3	1:A:329:GLU:HG2	1.75	0.67
1:A:565:GLU:HG2	3:A:655:HOH:O	1.93	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:A:90:GLU:O	1:A:94:GLU:HB2	1.93	0.67
1:B:528:GLY:HA2	1:B:533:ASP:HB2	1.77	0.67
1:A:193:VAL:H	1:A:286:THR:HG23	1.58	0.67
1:C:337:PRO:HG3	1:C:355:LEU:HD12	1.77	0.67
1:A:344:PRO:HD2	1:A:347:GLN:HG3	1.77	0.67
1:C:217:ARG:HH11	1:C:217:ARG:HG2	1.58	0.67
1:B:352:VAL:O	1:B:353:LYS:HG2	1.94	0.66
1:A:527:LYS:HG2	1:A:528:GLY:N	2.11	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: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:A:572:ARG:HD2	1:B:253:ASN:HB3	1.78	0.66
1:C:352:VAL:O	1:C:353:LYS:HG2	1.95	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:B:90:GLU:O	1:B:94:GLU:HB2	1.96	0.65
1:C:57:GLY:HA2	1:C:160:ILE:HG12	1.78	0.65
1:C:59:MET:CE	1:C:64:TYR:HA	2.27	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:B:337:PRO:HG3	1:B:355:LEU:HD12	1.80	0.64
1:C:372:ILE:HG13	1:C:386:ARG:HH22	1.62	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:A:231:LYS:HB2	1:A:234:ASP:HB2	1.79	0.63
1:C:115:ALA:HA	1:C:163:VAL:HG13	1.81	0.63
1:C:395:GLN:O	1:C:426:ARG:NH1	2.30	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:B:392:ARG:HG3	1:B:392:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ARG:HB3	1:C:347:GLN:HB2	1.82	0.62
1:C:546:VAL:HG11	1:C:556:ILE:HD13	1.81	0.62
1:B:331:GLN:NE2	1:B:344:PRO:HB3	2.14	0.62
1:C:344:PRO:HD2	1:C:347:GLN:HG3	1.81	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: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:B:344:PRO:HD2	1:B:347:GLN:HG3	1.82	0.62
1:C:159:LYS:NZ	3:C:578:HOH:O	2.32	0.61
1:B:55:LEU:HD11	1:B:57:GLY:O	2.00	0.61
1:B:343:ARG:HB3	1:B:347:GLN:HB2	1.82	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:A:372:ILE:HG13	1:A:386:ARG:HH22	1.65	0.61
1:A:528:GLY:HA2	1:A:533:ASP:HB2	1.82	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:C:60:ASN:HA	1:C:157:GLY:HA3	1.82	0.61
1:C:372:ILE:HG13	1:C:386:ARG:NH2	2.15	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:A:27:GLU:O	1:A:31:LEU:HG	2.03	0.59
1:C:204:ARG:HD3	1:C:378:TYR:CZ	2.37	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:199:ARG:HH11	1:B:265:MET:HE1	1.67	0.58
1:B:339:THR:HG22	1:B:341:GLU:OE2	2.03	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:HG22	1:A:122:ILE:O	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: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:C:373:PRO:HB3	1:C:375:TRP:CD1	2.39	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:73:LEU:HG	1:A:79:PHE:CB	2.34	0.57
1:A:572:ARG:NH2	3:A:651:HOH:O	2.37	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: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:C:339:THR:HG22	1:C:341:GLU:OE2	2.06	0.56
1:B:201:PRO:O	1:B:202:MET:HB2	2.06	0.56
1:A:194:VAL:HG22	1:A:287:HIS:HB2	1.87	0.56
1:A:204:ARG:HD3	1:A:378:TYR:OH	2.06	0.56
1:A:546:VAL:HG11	1:A:556:ILE:CG2	2.36	0.56
1:B:57:GLY:HA2	1:B:160:ILE:HG12	1.87	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: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:B:451:ARG:NH2	2:B:575:PPS:N1	2.51	0.55
1:C:417:GLN:OE1	1:C:430:LEU:HD22	2.07	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:A:86:ASP:OD2	1:A:152:LYS:HG2	2.06	0.55
1:A:527:LYS:HG2	1:A:528:GLY:H	1.70	0.55
1:C:336:LEU:HD22	1:C:352:VAL:CG1	2.35	0.55
1:C:199:ARG:HH11	1:C:265:MET:HE3	1.71	0.55
1:C:336:LEU:O	1:C:340:ASP:N	2.31	0.55
1:B:159:LYS:N	1:B:159:LYS:HE2	2.21	0.55
1:A:190:TRP:CZ3	1:A:257:VAL:HG23	2.43	0.54
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: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:B:286:THR:OG1	1:B:287:HIS:CD2	2.53	0.54
1:C:59:MET:HE3	1:C:64:TYR:CA	2.31	0.54
1:B:80:SER:HB2	1:B:271:ARG:HD3	1.90	0.54
1:B:123:TYR:CE1	1:B:155:TYR:HB2	2.43	0.54
1:C:330:PHE:CD1	1:C:330:PHE:C	2.81	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:292:ARG:NH2	1:A:309:PRO:HB3	2.23	0.53
1:A:331:GLN:O	1:A:331:GLN:HG3	2.08	0.53
1:A:372:ILE:HG13	1:A:386:ARG:NH2	2.22	0.53
1:B:331:GLN:O	1:B:331:GLN:HG3	2.08	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: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:C:204:ARG:HD3	1:C:378:TYR:CE1	2.44	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:176:TYR:CD2	1:B:181:LEU:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:HB1	1:B:219:ALA:O	2.09	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:423:GLN:HE21	1:B:425:GLY:N	1.91	0.53
1:C:331:GLN:O	1:C:331:GLN:HG3	2.08	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:A:176:TYR:CG	1:A:181:LEU:HD13	2.45	0.52
1:B:107:ASP:HB2	1:B:114:LEU:HD11	1.92	0.52
1:C:250:ARG:NE	1:C:378:TYR:CD2	2.77	0.52
1:A:22:ALA:O	1:A:25:ALA:HB3	2.09	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:275:TRP:O	1:A:279:ILE:HG13	2.10	0.52
1:B:527:LYS:HG2	1:B:528:GLY:H	1.73	0.52
1:A:48:MET:CE	1:A:162:ALA:HA	2.40	0.52
1:C:570:LEU:O	1:C:571:GLU:C	2.48	0.52
1:A:140:GLU:CD	1:A:300:ASN:HB2	2.30	0.52
1:A:281:LYS:HB2	1:A:325:ILE:HD12	1.92	0.52
1:A:330:PHE:CD1	1:A:330:PHE:C	2.83	0.52
1:B:2:ALA:HA	3:B:617:HOH:O	2.09	0.52
1:B:90:GLU:OE1	1:B:90:GLU:N	2.35	0.52
1:B:272:GLU:HG2	1:B:276:HIS:NE2	2.24	0.52
1:A:373:PRO:HB3	1:A:375:TRP:CD1	2.45	0.52
1:C:336:LEU:HD11	1:C:343:ARG:HD2	1.92	0.52
1:B:297:PRO:HB2	1:B:306:PHE:CD1	2.44	0.52
1:B:336:LEU:HD22	1:B:352:VAL:CG1	2.40	0.52
1:B:330:PHE:CD1	1:B:330:PHE:C	2.83	0.52
1:A:291:GLY:HA3	1:A:330:PHE:CE2	2.44	0.51
1:A:423:GLN:HE21	1:A:425:GLY:N	1.98	0.51
1:A:107:ASP:HB2	1:A:114:LEU:HD11	1.92	0.51
1:C:194:VAL:HA	1:C:287:HIS:HB2	1.93	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:B:546:VAL:HG11	1:B:556:ILE:HG23	1.92	0.51
1:C:207:ARG:O	1:C:207:ARG:HD3	2.10	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
1:C:423:GLN:HE22	1:C:425:GLY:HA3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLY:HA2	1:B:160:ILE:CG1	2.40	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:C:212:ARG:NH2	1:C:342:TYR:HB2	2.24	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:102:ARG:NH2	1:B:161:GLU:OE1	2.44	0.51
1:B:121:ASP:OD1	1:B:123:TYR:CD2	2.64	0.51
1:B:166:LEU:HD12	1:B:166:LEU:H	1.76	0.51
1:B:344:PRO:HD2	1:B:347:GLN:CG	2.39	0.51
1:B:342:TYR:N	1:B:342:TYR:CD1	2.78	0.50
1:A:86:ASP:HB2	1:A:152:LYS:HB2	1.94	0.50
1:B:60:ASN:HA	1:B:157:GLY:HA3	1.93	0.50
1:A:200:ASN:HB3	1:A:201:PRO:HD2	1.93	0.50
1:A:114:LEU:O	1:A:163:VAL:HG13	2.11	0.50
1:B:392:ARG:HG3	1:B:392:ARG:NH1	2.27	0.50
1:B:477:ILE:HG22	1:B:479:PRO:HG3	1.93	0.50
1:A:140:GLU:O	1:A:141:HIS:C	2.50	0.50
1:A:330:PHE:HD1	1:A:332:MET:H	1.59	0.50
1:B:425:GLY:HA2	1:B:573:GLN:HE22	1.77	0.50
1:C:3:ASN:ND2	3:C:634:HOH:O	2.44	0.50
1:C:204:ARG:NH1	1:C:204:ARG:HG2	2.26	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:A:73:LEU:HG	1:A:79:PHE:HB2	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:C:225:PRO:HD2	1:C:259:GLY:O	2.12	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:C:330:PHE:HD1	1:C:332:MET:H	1.60	0.50
1:A:436:VAL:HG11	1:A:458:ILE:HD11	1.94	0.49
1:B:43:ASP:O	1:B:47:ILE:HG13	2.11	0.49
1:B:65:ASP:O	1:B:69:GLU:HG2	2.12	0.49
1:A:160:ILE:CG2	1:A:161:GLU:N	2.74	0.49
1:B:52:PHE:O	1:B:53:SER:C	2.51	0.49
1:A:36:LEU:HB3	1:A:40:GLN:HB2	1.95	0.49
1:A:261:LEU:HD23	1:A:280:ARG:NH2	2.27	0.49
1:A:336:LEU:HD11	1:A:343:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HB2	1:B:339:THR:HB	1.92	0.49
1:B:417:GLN:OE1	1:B:430:LEU:HD22	2.12	0.49
1:C:299:SER:HB2	1:C:304:GLU:O	2.11	0.49
1:A:388:SER:HB3	3:A:642:HOH:O	2.11	0.49
1:A:361:GLU:O	1:A:365:ARG:HG3	2.12	0.49
1:B:92:ILE:HG23	1:B:97:LEU:HB2	1.95	0.49
1:B:336:LEU:HD11	1:B:343:ARG:HD2	1.95	0.49
1:B:360:THR:O	1:B:364:ARG:HB2	2.12	0.49
1:A:126:ASP:O	1:A:128:THR:N	2.46	0.49
1:A:339:THR:O	1:A:340:ASP:HB3	2.13	0.49
1:A:546:VAL:HG11	1:A:556:ILE:HG23	1.95	0.49
1:A:570:LEU:O	1:A:571:GLU:C	2.51	0.49
1:A:93:ASP:O	1:A:96:LYS:N	2.43	0.49
1:A:364:ARG:HA	1:A:367:ARG:HD3	1.95	0.49
1:C:320:LYS:CE	1:C:326:GLU:HG2	2.43	0.49
1:A:204:ARG:HD3	1:A:378:TYR:CE1	2.47	0.49
1:A:317:GLU:HA	1:A:320:LYS:HB2	1.95	0.49
1:A:336:LEU:HD22	1:A:352:VAL:CG1	2.42	0.49
1:C:115:ALA:HB1	1:C:161:GLU:O	2.13	0.49
1:B:528:GLY:O	1:B:534:ASP:HB2	2.12	0.49
1:A:134:VAL:HG22	1:A:271:ARG:NH1	2.28	0.49
1:C:59:MET:CE	1:C:82:PRO:HA	2.42	0.49
1:C:270:PRO:HB3	1:C:315:ALA:HB2	1.94	0.48
1:A:6:HIS:HB3	1:A:53:SER:O	2.12	0.48
1:A:115:ALA:HA	1:A:163:VAL:HG12	1.94	0.48
1:C:159:LYS:HE2	1:C:159:LYS:N	2.29	0.48
2:C:576:PPS:H5'2	2:C:576:PPS:N3	2.29	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:A:362:LEU:HD22	1:A:376:PHE:CE2	2.48	0.48
1:B:339:THR:O	1:B:340:ASP:HB3	2.14	0.48
1:A:39:ARG:HD2	3:A:626:HOH:O	2.13	0.48
1:A:449:GLU:HG3	3:A:657:HOH:O	2.13	0.48
1:B:330:PHE:HD1	1:B:332:MET:H	1.60	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:A:11:LYS:HD2	1:A:11:LYS:N	2.29	0.48
1:A:71:ASN:OD1	1:A:80:SER:HB3	2.13	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:272:GLU:HG3	1:B:275:TRP:HE3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:GLU:CD	1:B:507:GLU:H	2.17	0.48
1:B:547:ASP:OD1	1:B:549:SER:HB2	2.13	0.48
1:C:207:ARG:NE	1:C:250:ARG:O	2.42	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:339:THR:O	1:C:340:ASP:HB3	2.14	0.48
1:C:534:ASP:OD2	1:C:535:PRO:HD2	2.13	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:197:GLN:HE22	1:A:226:VAL:HG21	1.79	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:171:TYR:CE1	1:A:241:VAL:HG11	2.49	0.48
1:B:11:LYS:N	1:B:11:LYS:HD2	2.27	0.48
1:A:392:ARG:HD2	1:A:569:PHE:CZ	2.49	0.48
1:B:21:GLN:HA	3:B:630:HOH:O	2.14	0.48
1:B:336:LEU:O	1:B:340:ASP:N	2.33	0.48
1:C:202:MET:HA	1:C:206:HIS:ND1	2.28	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:A:114:LEU:C	1:A:163:VAL:HG13	2.33	0.47
1:B:302:LYS:HE3	1:B:304:GLU:OE2	2.13	0.47
1:B:346:ASP:C	1:B:348:VAL:H	2.18	0.47
1:C:330:PHE:CD1	1:C:330:PHE:O	2.67	0.47
1:C:378:TYR:HB3	1:C:380:GLU:OE1	2.13	0.47
1:C:392:ARG:HD2	1:C:569:PHE:CZ	2.50	0.47
1:C:423:GLN:HE21	1:C:425:GLY:N	2.02	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:290:VAL:HG23	1:C:327:VAL:HG13	1.96	0.47
1:C:448:ARG:NH1	1:C:482:GLU:OE1	2.47	0.47
1:A:432:LEU:HD23	1:A:475:ALA:HB3	1.95	0.47
1:A:507:GLU:CD	1:A:507:GLU:H	2.16	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:C:80:SER:HB2	1:C:271:ARG:HD3	1.97	0.47
1:C:208:GLU:O	1:C:212:ARG:CG	2.57	0.47
1:A:47:ILE:HD11	1:A:83:ILE:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:O	1:A:492:SER:OG	2.29	0.47
1:B:263:LEU:HD11	1:B:275:TRP:CH2	2.49	0.47
1:C:61:GLN:NE2	1:C:65:ASP:OD2	2.46	0.47
1:C:290:VAL:CG2	1:C:327:VAL:HG13	2.45	0.47
1:C:1:MET:CG	1:C:2:ALA:N	2.78	0.47
1:C:546:VAL:HG21	1:C:556:ILE:HG23	1.97	0.47
1:B:122:ILE:O	1:B:122:ILE:HG22	2.15	0.47
1:B:190:TRP:CH2	1:B:257:VAL:HG23	2.50	0.47
1:A:140:GLU:CD	1:A:301:SER:H	2.18	0.46
1:B:127:LYS:HD3	1:B:147:LEU:O	2.14	0.46
1:B:448:ARG:NH1	1:B:482:GLU:OE1	2.47	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: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:361:GLU:O	1:B:365:ARG:HG3	2.15	0.46
1:B:519:ALA:HB3	3:B:674:HOH:O	2.15	0.46
1:C:546:VAL:HG11	1:C:556:ILE:HG23	1.97	0.46
1:B:48:MET:HG2	1:B:162:ALA:HB2	1.96	0.46
1:B:339:THR:HG22	1:B:341:GLU:CD	2.36	0.46
1:C:206:HIS:O	1:C:209:LEU:HB3	2.15	0.46
1:B:364:ARG:HA	1:B:367:ARG:HD3	1.96	0.46
1:A:171:TYR:HB3	1:A:174:LEU:HD12	1.97	0.46
1:A:199:ARG:NH1	1:A:265:MET:CE	2.78	0.46
1:B:452:HIS:O	1:B:456:GLN:HG3	2.16	0.46
1:C:203:HIS:HE1	1:C:385:LEU:CD1	2.29	0.46
1:A:5:PRO:O	1:A:281:LYS:HE3	2.16	0.46
1:A:40:GLN:NE2	1:A:85:LEU:HD12	2.30	0.46
1:A:208:GLU:OE2	1:A:208:GLU:HA	2.15	0.46
1:A:346:ASP:C	1:A:348:VAL:H	2.19	0.46
1:A:378:TYR:HB3	1:A:380:GLU:OE1	2.16	0.46
1:B:40:GLN:NE2	1:B:85:LEU:HD12	2.30	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:A:217:ARG:HH11	1:A:217:ARG:HG2	1.81	0.46
1:C:266:ARG:O	1:C:267:MET:HB2	2.16	0.46
1:C:362:LEU:HD22	1:C:376:PHE:CE2	2.50	0.46
1:B:546:VAL:HG11	1:B:556:ILE:HG21	1.96	0.46
1:C:346:ASP:C	1:C:348:VAL:H	2.18	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:A:24:LEU:HD23	1:A:116:ILE:HD12	1.98	0.45
1:A:113:ASN:O	1:A:164:ASN:HB2	2.17	0.45
1:C:263:LEU:HD11	1:C:275:TRP:CH2	2.51	0.45
1:C:312:ALA:HB3	3:C:620:HOH:O	2.16	0.45
1:C:339:THR:HG22	1:C:341:GLU:CD	2.37	0.45
1:A:109:ARG:NE	1:A:229:LEU:HD13	2.31	0.45
1:A:119:ILE:CG2	1:A:120:ASP:N	2.79	0.45
1:A:292:ARG:CZ	1:A:292:ARG:HB3	2.46	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:C:333:VAL:HG23	1:C:342:TYR:HB3	1.99	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:A:72:ARG:NH1	1:A:76:GLY:O	2.48	0.45
1:B:88:SER:O	1:B:92:ILE:HG13	2.17	0.45
1:A:349:PRO:O	1:A:352:VAL:HG23	2.17	0.45
1:B:441:SER:OG	1:B:454:ASN:ND2	2.48	0.45
1:C:344:PRO:C	1:C:346:ASP:H	2.20	0.45
1:C:546:VAL:CG1	1:C:556:ILE:CD1	2.94	0.45
1:A:36:LEU:HD21	1:A:105:LEU:HD22	1.98	0.45
1:A:66:ARG:O	1:A:70:ASP:HB2	2.16	0.45
1:A:270:PRO:HG3	1:A:311:ASP:C	2.37	0.45
1:A:313:GLN:HB3	1:A:329:GLU:CG	2.43	0.45
1:B:344:PRO:C	1:B:346:ASP:H	2.20	0.45
1:C:197:GLN:HE22	1:C:265:MET:HE2	1.80	0.45
1:C:349:PRO:O	1:C:352:VAL:HG23	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: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:357:ILE:HB	1:C:376:PHE:CE1	2.52	0.45
1:B:362:LEU:HD22	1:B:376:PHE:CE2	2.52	0.44
1:C:203:HIS:N	1:C:206:HIS:ND1	2.47	0.44
1:B:330:PHE:CD1	1:B:330:PHE:O	2.70	0.44
1:B:477:ILE:CG2	1:B:479:PRO:HG3	2.46	0.44
1:A:88:SER:O	1:A:92:ILE:HG13	2.16	0.44
1:A:129:LYS:O	1:A:130:GLU:C	2.55	0.44
1:C:204:ARG:HG2	1:C:204:ARG:HH11	1.83	0.44
1:C:214:ALA:HB3	1:C:255:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ARG:HH21	1:C:379:PRO:HD2	1.82	0.44
1:C:392:ARG:NH1	1:C:567:GLN:O	2.50	0.44
1:A:36:LEU:HD22	1:A:85:LEU:HD13	1.99	0.44
1:A:423:GLN:NE2	1:A:425:GLY:HA3	2.32	0.44
1:A:447:THR:O	1:A:448:ARG:C	2.55	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:A:109:ARG:HD3	1:A:229:LEU:HD13	1.99	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:B:443:GLU:HB2	3:B:654:HOH:O	2.16	0.44
1:C:90:GLU:CD	1:C:90:GLU:H	2.21	0.44
1:C:255:MET:O	1:C:255:MET:HG2	2.17	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:CD1	1:B:108:PHE:C	2.91	0.44
1:A:133:LEU:N	1:A:133:LEU:HD23	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:A:190:TRP:CH2	1:A:257:VAL:HG23	2.52	0.44
1:A:226:VAL:HG12	1:A:227:VAL:N	2.33	0.44
1:B:90:GLU:H	1:B:90:GLU:CD	2.20	0.44
1:B:437:ARG:HD2	1:B:437:ARG:HA	1.87	0.44
1:C:48:MET:HE1	1:C:164:ASN:O	2.17	0.44
1:C:190:TRP:CZ3	1:C:257:VAL:HG23	2.52	0.44
1:C:510:GLU:HG2	1:C:518:TYR:CG	2.53	0.44
1:C:546:VAL:HG11	1:C:556:ILE:HG21	2.00	0.44
1:A:339:THR:HG22	1:A:341:GLU:CD	2.38	0.43
1:A:448:ARG:NH1	1:A:482:GLU:OE1	2.50	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:C:510:GLU:HG2	1:C:518:TYR:CD2	2.53	0.43
1:A:31:LEU:HD22	1:A:102:ARG:O	2.17	0.43
1:A:333:VAL:HG23	1:A:342:TYR:HB3	2.00	0.43
1:B:451:ARG:HH12	2:B:575:PPS:C2	2.31	0.43
1:A:26:ALA:O	1:A:29:GLU:HB2	2.18	0.43
1:A:292:ARG:HH21	1:A:309:PRO:HB3	1.82	0.43
1:A:520:ALA:HB1	1:A:525:GLU:HB2	2.00	0.43
1:A:528:GLY:O	1:A:534:ASP:HB2	2.19	0.43
1:C:204:ARG:NH2	1:C:342:TYR:OH	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:GLY:HA2	1:C:297:PRO:HD3	1.81	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:B:81:MET:SD	1:B:82:PRO:HD2	2.58	0.43
1:C:390:PRO:HA	1:C:391:PRO:HD3	1.80	0.43
1:A:274:ILE:HD11	1:A:315:ALA:O	2.19	0.43
1:A:452:HIS:O	1:A:456:GLN:HG3	2.18	0.43
1:B:44:LEU:HA	1:B:47:ILE:HD12	2.01	0.43
1:B:98:GLN:O	1:B:99:ALA:C	2.55	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:A:16:ARG:O	1:A:18:ALA:N	2.51	0.43
1:A:126:ASP:C	1:A:128:THR:H	2.22	0.43
1:A:337:PRO:HG2	1:A:355:LEU:HG	2.00	0.43
1:A:572:ARG:HD2	1:B:253:ASN:OD1	2.19	0.43
1:B:202:MET:HA	1:B:206:HIS:ND1	2.33	0.43
1:B:214:ALA:HB2	1:B:221:VAL:CG2	2.49	0.43
1:C:334:THR:OG1	1:C:335:TYR:N	2.52	0.43
1:A:562:LEU:HA	1:A:562:LEU:HD23	1.79	0.43
1:C:207:ARG:HD3	1:C:207:ARG:C	2.39	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:1:MET:CE	1:A:5:PRO:HD3	2.49	0.43
1:A:193:VAL:H	1:A:286:THR:CG2	2.29	0.43
1:A:390:PRO:HA	1:A:391:PRO:HD3	1.80	0.43
1:A:425:GLY:HA2	1:A:573:GLN:HE22	1.84	0.43
1:A:71:ASN:OD1	1:A:80:SER:CB	2.67	0.42
1:B:103:ILE:O	1:B:116:ILE:HA	2.19	0.42
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:C:544:LEU:HD11	1:C:559:GLU:OE2	2.19	0.42
1:A:74:ALA:O	1:A:76:GLY:N	2.50	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: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:C:512:SER:O	1:C:514:LYS:HG3	2.18	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:C:212:ARG:NH2	1:C:342:TYR:HD1	2.17	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:A:39:ARG:NH1	1:A:266:ARG:HG3	2.34	0.42
1:A:572:ARG:HD2	1:B:253:ASN:CB	2.48	0.42
1:B:337:PRO:CD	1:B:353:LYS:CB	2.89	0.42
1:B:512:SER:O	1:B:514:LYS:HG3	2.20	0.42
1:C:1:MET:HG3	1:C:2:ALA:H	1.83	0.42
1:A:59:MET:HE3	1:A:67:VAL:HG21	1.99	0.42
1:A:89:GLN:HA	1:A:92:ILE:HD12	2.02	0.42
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.76	0.42
1:A:273:ALA:O	1:A:276:HIS:HB2	2.20	0.42
1:B:41:LEU:HA	1:B:41:LEU:HD23	1.65	0.42
1:B:562:LEU:HD23	1:B:562:LEU:HA	1.78	0.42
1:C:102:ARG:NH2	1:C:161:GLU:OE1	2.52	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:C:204:ARG:H	1:C:377:SER:HA	1.84	0.42
1:A:292:ARG:O	1:A:293:ASP:HB2	2.19	0.42
1:B:117:LEU:C	1:B:117:LEU:CD2	2.86	0.42
1:B:192:ARG:HB3	1:B:219:ALA:HB2	2.02	0.42
1:B:250:ARG:HG3	1:B:378:TYR:CD2	2.55	0.42
1:B:299:SER:HA	1:B:304:GLU:O	2.19	0.42
1:B:451:ARG:HH12	2:B:575:PPS:H2	1.85	0.42
1:C:36:LEU:HB2	1:C:41:LEU:HG	2.02	0.42
1:A:138:ASP:HA	1:A:139:PRO:HD3	1.78	0.42
1:A:251:TYR:O	1:A:252:PRO:C	2.57	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:138:ASP:OD2	1:A:138:ASP:C	2.59	0.41
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:B:546:VAL:HG21	1:B:556:ILE:HG23	2.02	0.41
1:C:57:GLY:HA2	1:C:160:ILE:HG13	2.01	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:CD	1:C:507:GLU:H	2.24	0.41
1:A:223:ILE:HD11	1:A:251:TYR:CE1	2.55	0.41
1:A:477:ILE:CG2	1:A:479:PRO:HG3	2.50	0.41
1:A:565:GLU:CB	3:A:655:HOH:O	2.68	0.41
1:C:98:GLN:HA	1:C:122:ILE:CD1	2.51	0.41
1:B:20:ARG:HD2	3:B:622:HOH:O	2.20	0.41
1:C:98:GLN:O	1:C:99:ALA:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD11	1:A:105:LEU:HB3	2.03	0.41
1:A:334:THR:OG1	1:A:335:TYR:N	2.53	0.41
1:A:477:ILE:HG22	1:A:479:PRO:HG3	2.02	0.41
1:B:337:PRO:HG3	1:B:355:LEU:CD1	2.49	0.41
1:A:362:LEU:HD22	1:A:376:PHE:HE2	1.85	0.41
1:B:48:MET:HE2	1:B:115:ALA:HB2	1.94	0.41
1:B:217:ARG:HG2	1:B:217:ARG:HH11	1.85	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:345:VAL:HG11	3:C:693:HOH:O	2.17	0.41
1:A:31:LEU:CD2	1:A:102:ARG:HB3	2.45	0.41
1:A:109:ARG:HH21	1:A:166:LEU:CD1	2.34	0.41
1:C:92:ILE:HA	1:C:97:LEU:HD12	2.02	0.41
1:C:337:PRO:HG3	1:C:355:LEU:CD1	2.47	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:B:313:GLN:NE2	1:B:329:GLU:HG2	2.35	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:A:153:GLU:HG2	1:A:154:PHE:CD2	2.55	0.41
1:A:440:LEU:O	1:A:457:ARG:HD3	2.21	0.41
1:B:131:ALA:HB1	1:B:144:ILE:CD1	2.50	0.41
1:B:392:ARG:NH1	1:B:567:GLN:O	2.52	0.41
1:B:447:THR:O	1:B:448:ARG:C	2.59	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:C:436:VAL:HG11	1:C:458:ILE:HD11	2.02	0.41
1:C:547:ASP:OD1	1:C:549:SER:HB2	2.21	0.41
1:B:86:ASP:HA	1:B:154:PHE:O	2.21	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: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:296:GLY:HA2	1:A:297:PRO:HD3	1.88	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:46:LEU:O	1:C:51:GLY:N	2.54	0.40
1:C:246:ALA:O	1:C:249:PRO:HD2	2.21	0.40
1:C:504:THR:HA	1:C:505:PRO:HD3	1.96	0.40
1:B:209:LEU:HD13	1:B:330:PHE:HB2	2.03	0.40
1:C:250:ARG:HG3	1:C:378:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:HB3	1:A:95:LYS:HB3	2.03	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:B:93:ASP:O	1:B:94:GLU:C	2.59	0.40
1:C:41:LEU:HD22	1:C:166:LEU:HD13	2.02	0.40
1:C:269:GLY:HA3	1:C:270:PRO:HD3	1.91	0.40
1:C:372:ILE:HA	1:C:373:PRO:HD3	1.84	0.40
1:C:447:THR:O	1:C:448:ARG:C	2.59	0.40
1:A:109:ARG:CD	1:A:229:LEU:HD13	2.51	0.40
1:A:512:SER:O	1:A:514:LYS:HG3	2.21	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:C:374:GLU:HG3	1:C:379:PRO:HD3	2.04	0.40
1:C:249:PRO:C	1:C:251:TYR:H	2.25	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

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%)	3 3
1	B	571/573 (100%)	513 (90%)	47 (8%)	11 (2%)	8 15
1	C	571/573 (100%)	517 (90%)	46 (8%)	8 (1%)	11 22
All	All	1713/1719 (100%)	1522 (89%)	149 (9%)	42 (2%)	5 9

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 (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	472/474 (100%)	438 (93%)	34 (7%)	14	29
1	B	472/474 (100%)	448 (95%)	24 (5%)	24	46
1	C	472/474 (100%)	452 (96%)	20 (4%)	30	55
All	All	1416/1422 (100%)	1338 (94%)	78 (6%)	21	43

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	-	29,33,33	1.60	5 (17%)	36,52,52	1.47	6 (16%)
2	PPS	B	575	-	29,33,33	1.69	7 (24%)	36,52,52	1.56	8 (22%)
2	PPS	C	576	-	29,33,33	1.77	5 (17%)	36,52,52	1.58	6 (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	-	-	1/11/37/37	0/3/3/3
2	PPS	B	575	-	-	3/11/37/37	0/3/3/3
2	PPS	C	576	-	-	0/11/37/37	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	576	PPS	O4'-C1'	6.35	1.49	1.40
2	B	575	PPS	O4'-C1'	5.38	1.48	1.40
2	A	574	PPS	O4'-C1'	5.31	1.47	1.40
2	B	575	PPS	C4-N3	3.04	1.39	1.35
2	C	576	PPS	C2-N1	2.97	1.39	1.33
2	B	575	PPS	C2-N1	2.63	1.38	1.33
2	C	576	PPS	P2-O6P	2.60	1.66	1.59
2	C	576	PPS	C8-N7	-2.57	1.30	1.34
2	A	574	PPS	C4-N3	2.51	1.39	1.35
2	A	574	PPS	C1'-N9	-2.39	1.44	1.49
2	A	574	PPS	C2-N1	2.38	1.38	1.33
2	B	575	PPS	C8-N7	-2.27	1.30	1.34
2	B	575	PPS	O5'-C5'	-2.15	1.36	1.44
2	B	575	PPS	C1'-N9	-2.05	1.44	1.49
2	A	574	PPS	C8-N7	-2.02	1.31	1.34
2	B	575	PPS	C2'-C3'	2.01	1.57	1.53
2	C	576	PPS	C4-N3	2.00	1.38	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	576	PPS	O4'-C1'-N9	4.08	114.15	108.75
2	A	574	PPS	C2'-C3'-C4'	-2.95	98.08	103.24
2	B	575	PPS	C5-C6-N1	-2.93	113.23	120.23
2	B	575	PPS	C5-C6-N6	2.74	124.49	120.31
2	C	576	PPS	O2P-P1-O1P	2.72	118.00	107.80
2	A	574	PPS	C5-C6-N1	-2.71	113.77	120.23
2	A	574	PPS	O2P-P1-O1P	2.63	117.67	107.80
2	B	575	PPS	C2'-C3'-C4'	-2.62	98.65	103.24
2	C	576	PPS	C5-C6-N1	-2.61	114.00	120.23
2	A	574	PPS	C5-C6-N6	2.56	124.21	120.31
2	B	575	PPS	O4'-C1'-N9	2.55	112.13	108.75
2	B	575	PPS	O2P-P1-O1P	2.41	116.82	107.80
2	C	576	PPS	O3'-C3'-C2'	-2.37	103.16	111.68
2	B	575	PPS	O6P-P2-O4P	-2.34	103.67	110.70
2	B	575	PPS	C1'-N9-C4	2.32	130.72	126.64
2	C	576	PPS	C1'-N9-C4	2.24	130.57	126.64
2	B	575	PPS	C4'-O4'-C1'	2.16	111.90	109.92
2	C	576	PPS	C5-C6-N6	2.12	123.54	120.31
2	A	574	PPS	C1'-N9-C4	2.06	130.25	126.64
2	A	574	PPS	O4'-C1'-N9	2.02	111.42	108.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	575	PPS	C3'-C4'-C5'-O5'
2	B	575	PPS	O4'-C4'-C5'-O5'
2	B	575	PPS	C2'-C3'-O3'-P1
2	A	574	PPS	C2'-C3'-O3'-P1

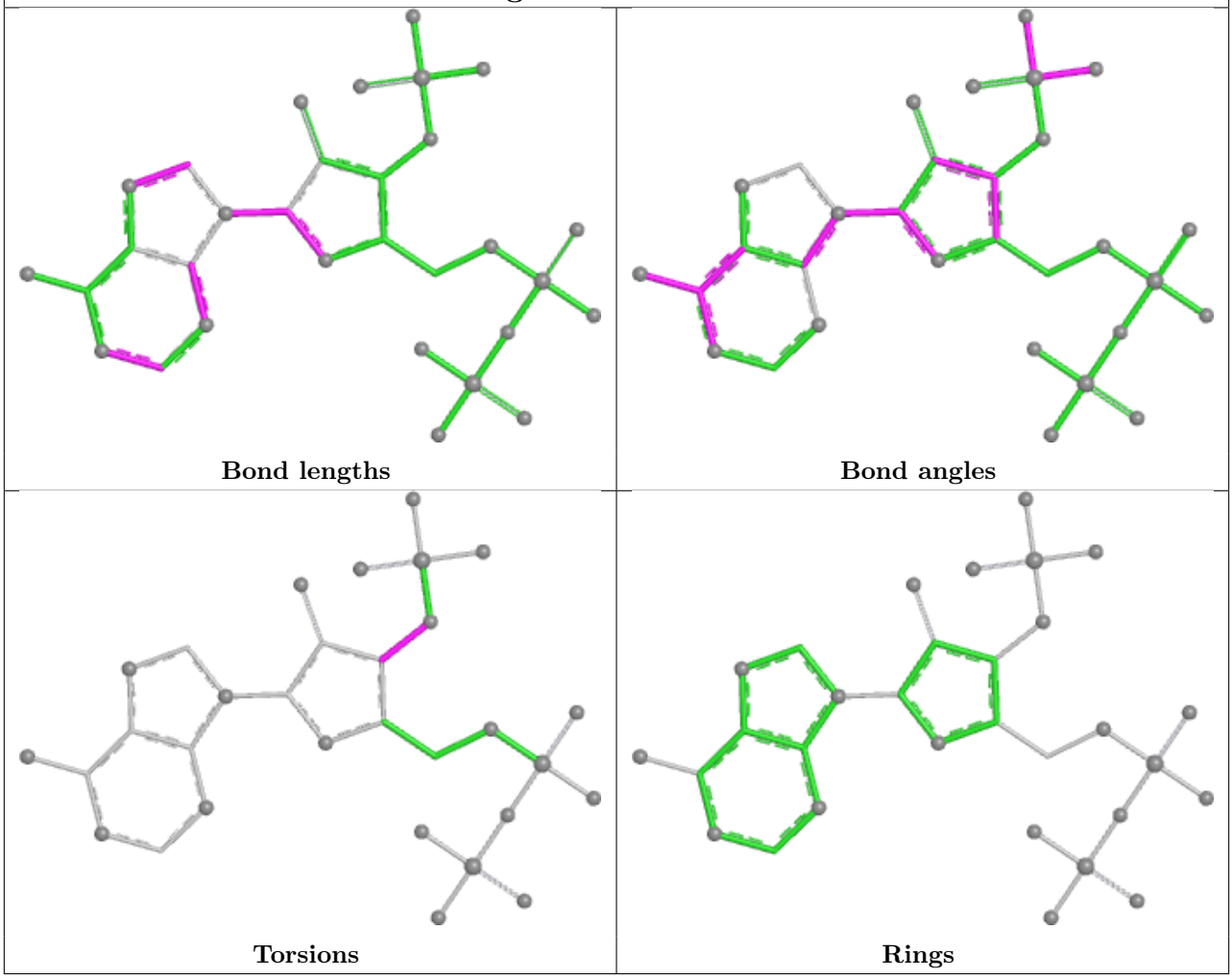
There are no ring outliers.

3 monomers are involved in 8 short contacts:

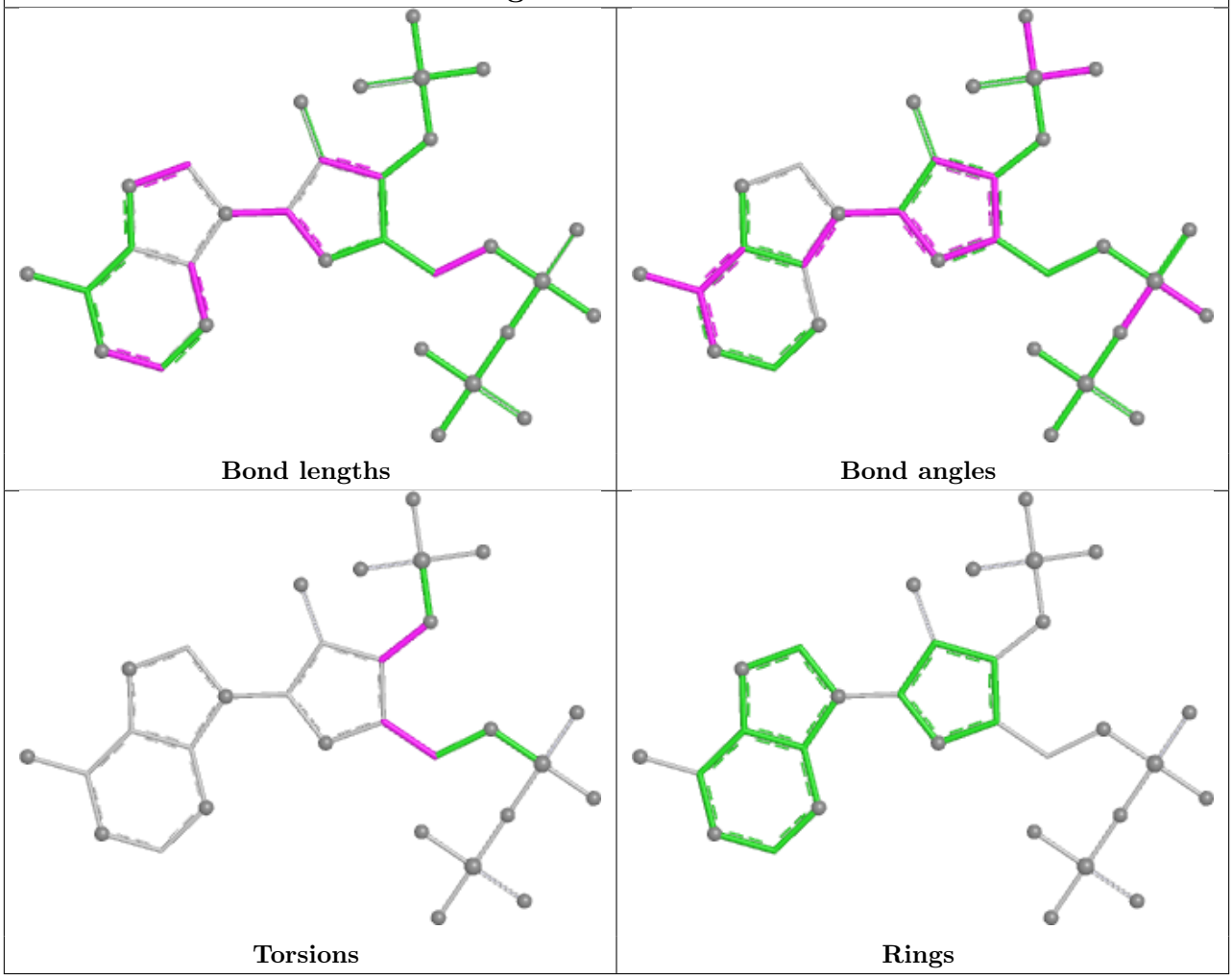
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	574	PPS	2	0
2	B	575	PPS	4	0
2	C	576	PPS	2	0

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.

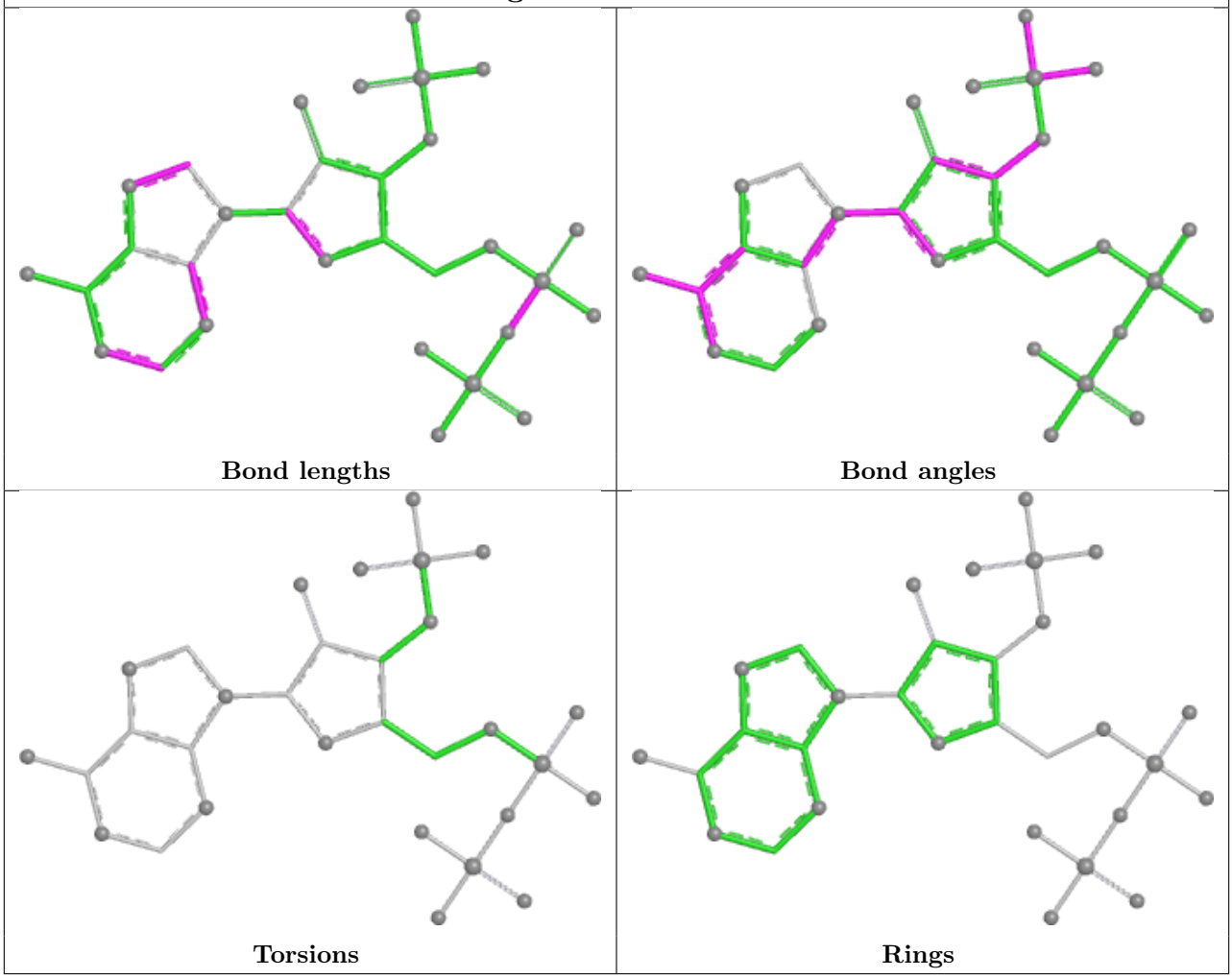
Ligand PPS A 574



Ligand PPS B 575



Ligand PPS C 576



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	573/573 (100%)	0.22	43 (7%)	14	10	30, 75, 129, 165	0
1	B	573/573 (100%)	-0.07	19 (3%)	46	39	30, 59, 102, 157	0
1	C	573/573 (100%)	-0.11	25 (4%)	34	27	29, 53, 122, 168	0
All	All	1719/1719 (100%)	0.02	87 (5%)	28	22	29, 60, 119, 168	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	GLU	9.1
1	C	350	ALA	7.8
1	B	349	PRO	7.2
1	C	348	VAL	7.1
1	C	1	MET	6.3
1	A	573	GLN	6.2
1	A	348	VAL	5.7
1	B	333	VAL	5.6
1	A	154	PHE	5.6
1	B	527	LYS	5.5
1	A	572	ARG	5.4
1	C	333	VAL	5.4
1	C	349	PRO	5.0
1	A	352	VAL	4.9
1	A	334	THR	4.9
1	C	352	VAL	4.7
1	A	350	ALA	4.7
1	A	1	MET	4.7
1	A	353	LYS	4.5
1	C	334	THR	4.3
1	C	339	THR	4.2
1	C	360	THR	4.1
1	A	349	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	573	GLN	3.9
1	C	343	ARG	3.9
1	A	360	THR	3.9
1	A	341	GLU	3.9
1	A	303	GLY	3.8
1	A	354	THR	3.8
1	B	352	VAL	3.8
1	A	345	VAL	3.7
1	A	305	ASP	3.5
1	C	340	ASP	3.4
1	A	332	MET	3.4
1	C	346	ASP	3.3
1	A	91	VAL	3.3
1	C	573	GLN	3.2
1	A	84	THR	3.2
1	C	372	ILE	3.1
1	A	339	THR	3.1
1	A	364	ARG	3.0
1	B	572	ARG	3.0
1	A	309	PRO	3.0
1	A	299	SER	3.0
1	A	300	ASN	3.0
1	B	347	GLN	3.0
1	B	523	ARG	3.0
1	A	304	GLU	2.9
1	B	348	VAL	2.9
1	B	343	ARG	2.8
1	A	82	PRO	2.8
1	A	333	VAL	2.8
1	C	347	GLN	2.8
1	C	572	ARG	2.8
1	C	2	ALA	2.7
1	A	310	TYR	2.7
1	A	70	ASP	2.7
1	B	334	THR	2.6
1	A	133	LEU	2.6
1	A	306	PHE	2.6
1	B	350	ALA	2.5
1	B	1	MET	2.5
1	A	139	PRO	2.5
1	C	353	LYS	2.5
1	B	540	GLU	2.5

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PPS	A	574	31/31	0.95	0.13	59,72,103,111	0

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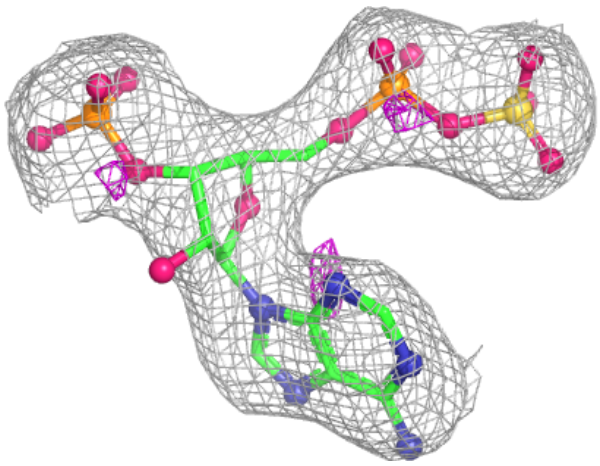
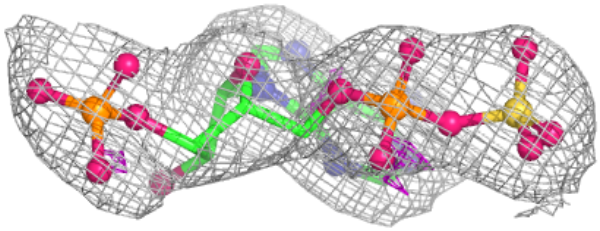
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PPS	B	575	31/31	0.95	0.14	50,68,96,97	0
2	PPS	C	576	31/31	0.97	0.11	41,59,89,98	0

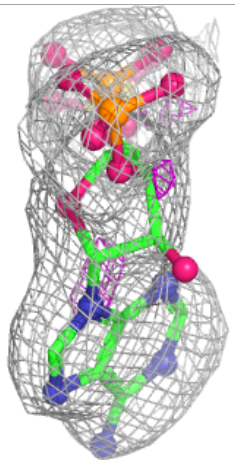
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PPS A 574:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

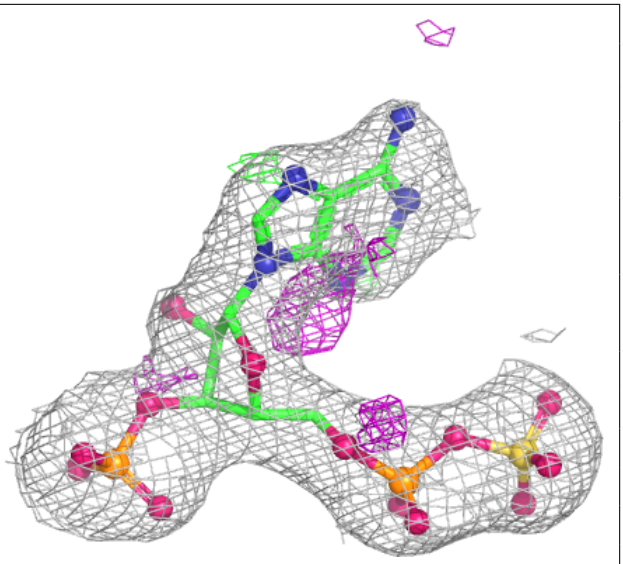


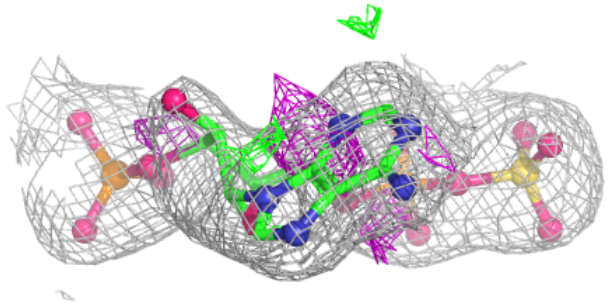


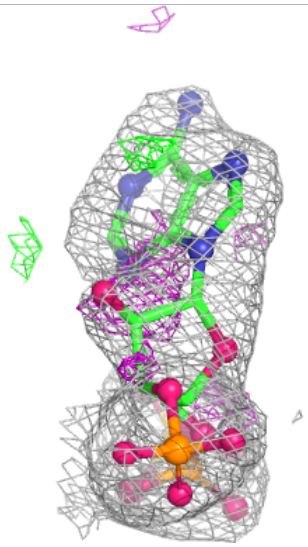


Electron density around PPS B 575:

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

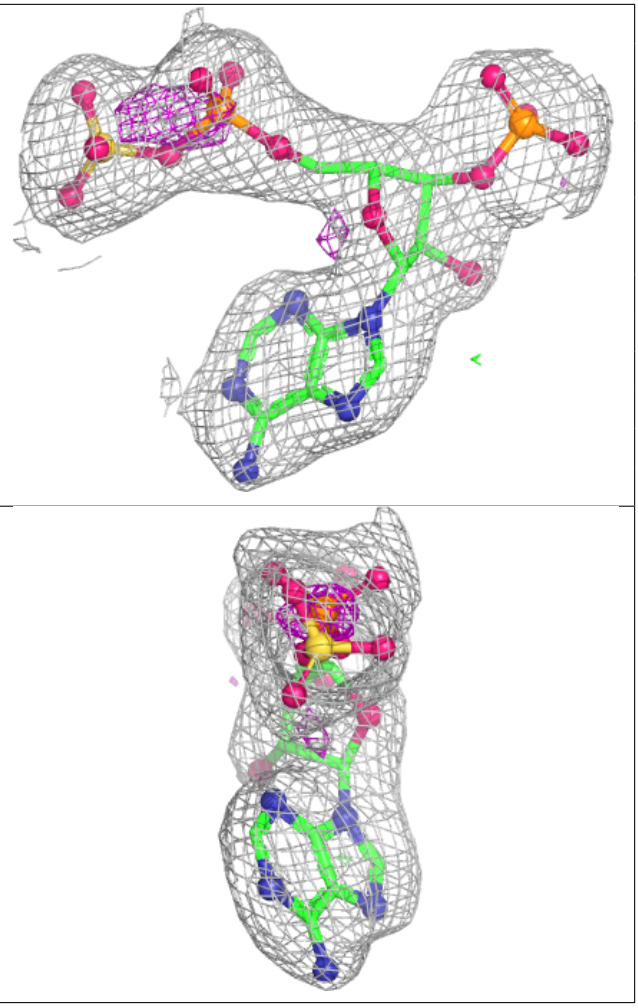






Electron density around PPS C 576:

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 (i)

There are no such residues in this entry.