Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 11:45 pm BST

PDB ID	:	2ZXF
Title	:	Crystal structure of human glycyl-trna synthetase (GLYRS) in complex with AP4A (cocrystallized with AP4A)
Authors	:	Guo, R.T.; Yang, X.L.; Schimmel, P.
Deposited on	:	2008-12-23
Resolution	:	3.40 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 following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.40 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	Percentile Ranks	Value
Rfree		0.288
Clashscore		47
Ramachandran outliers		10.3%
Sidechain outliers		10.9%
RSRZ outliers		11.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
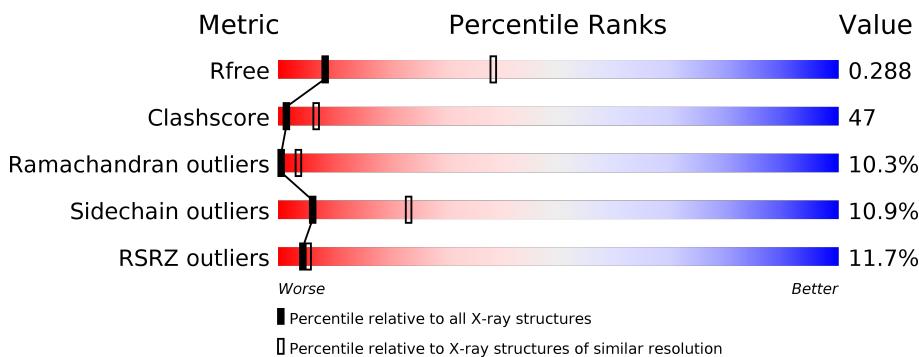
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	693	9% — 24% / 42% / 10% / 24%
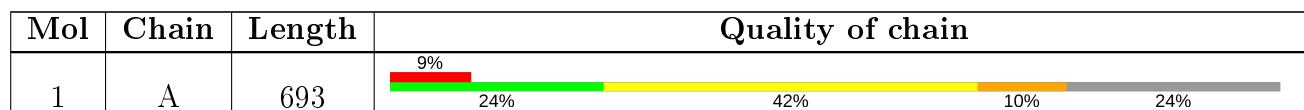
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	B4P	A	1101	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4352 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 Glycyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	530	4228	2689	728	787	24	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	686	LEU	-	EXPRESSION TAG	UNP P41250
A	687	GLU	-	EXPRESSION TAG	UNP P41250
A	688	HIS	-	EXPRESSION TAG	UNP P41250
A	689	HIS	-	EXPRESSION TAG	UNP P41250
A	690	HIS	-	EXPRESSION TAG	UNP P41250
A	691	HIS	-	EXPRESSION TAG	UNP P41250
A	692	HIS	-	EXPRESSION TAG	UNP P41250
A	693	HIS	-	EXPRESSION TAG	UNP P41250

- Molecule 2 is BIS(ADENOSINE)-5'-TETRAPHOSPHATE (three-letter code: B4P) (formula: $C_{20}H_{28}N_{10}O_{19}P_4$).

B4P
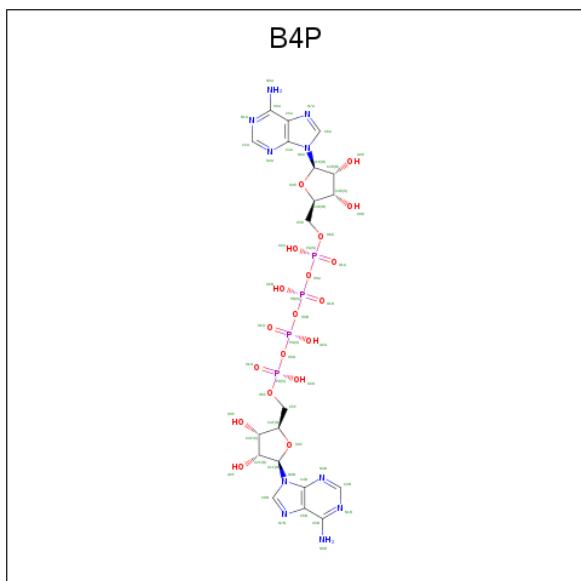
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	20	10	19	4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	71	71	71	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Glycyl-tRNA synthetase

L655 A656 N657 I660 T661 W662 A663 D664 V665 R668 Y669 P670 L671 F672 E673 GLY GLN GLU THR GLY LYS LYS GLU THR ILE GLU GLU LEU GLU HIS HIS HIS HIS HIS HIS
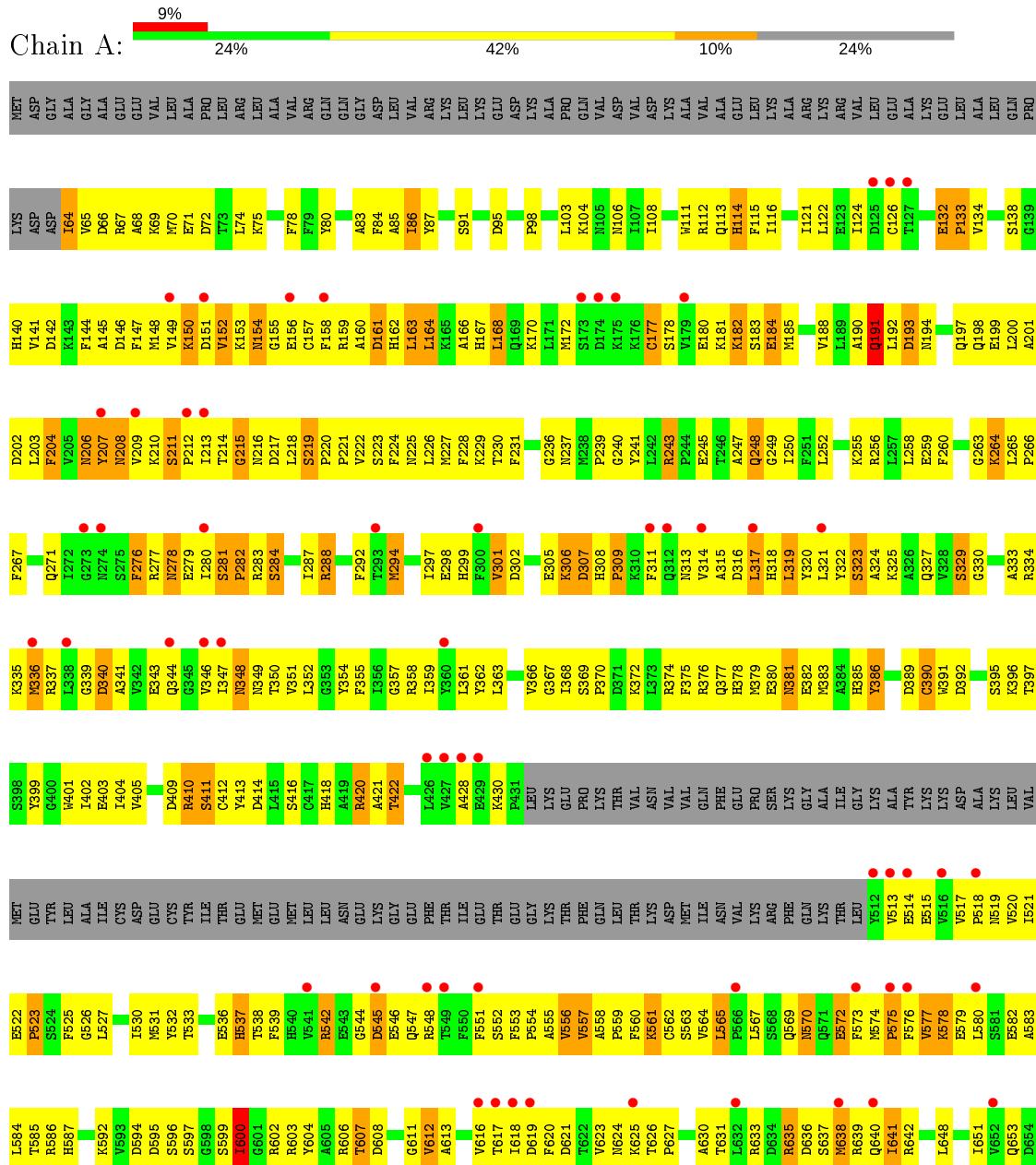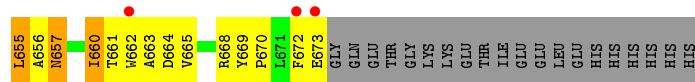
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	121.30Å 137.03Å 132.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 45.41 – 3.39	Depositor EDS
% Data completeness (in resolution range)	86.4 (50.00-3.40) 86.1 (45.41-3.39)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	6.22 (at 3.40Å)	Xtriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.244 , 0.288 0.239 , 0.288	Depositor DCC
R_{free} test set	682 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	121.5	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 117.7	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4352	wwPDB-VP
Average B, all atoms (Å^2)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: B4P

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	0.33	0/4326	0.68	0/5847

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	4228	0	4145	393	0
2	A	53	0	24	4	0
3	A	71	0	0	1	0
All	All	4352	0	4169	395	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 47.

All (395) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:THR:HB	1:A:631:THR:HB	1.24	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HD12	1:A:214:THR:HG22	1.40	1.03
1:A:148:MET:HB2	1:A:280:ILE:HD13	1.49	0.94
1:A:154:ASN:HA	3:A:702:HOH:O	1.70	0.92
1:A:664:ASP:HB3	1:A:668:ARG:HH12	1.36	0.91
1:A:145:ALA:HB2	1:A:225:ASN:HA	1.52	0.88
1:A:145:ALA:HB1	1:A:224:PHE:O	1.74	0.86
1:A:305:GLU:O	1:A:307:ASP:N	2.09	0.85
1:A:211:SER:H	1:A:218:LEU:CD1	1.90	0.84
1:A:633:ARG:HB2	1:A:640:GLN:HG2	1.58	0.84
1:A:193:ASP:HB3	1:A:382:GLU:HG3	1.59	0.83
1:A:620:PHE:HB3	1:A:624:ASN:HD21	1.43	0.83
1:A:211:SER:H	1:A:218:LEU:HD13	1.44	0.82
1:A:265:LEU:HD21	1:A:518:PRO:HG3	1.61	0.81
1:A:194:ASN:HD21	1:A:379:MET:HB3	1.44	0.81
1:A:132:GLU:HB3	1:A:133:PRO:HD3	1.63	0.79
1:A:209:VAL:HG12	1:A:218:LEU:HD22	1.65	0.78
1:A:567:LEU:HD13	1:A:619:ASP:HA	1.66	0.78
1:A:74:LEU:HD13	1:A:80:TYR:HE1	1.49	0.78
1:A:617:THR:HB	1:A:631:THR:CB	2.11	0.78
1:A:163:LEU:HD21	1:A:212:PRO:HD3	1.65	0.77
1:A:201:ALA:HA	1:A:221:PRO:HG3	1.64	0.77
1:A:104:LYS:O	1:A:108:ILE:HG13	1.85	0.77
1:A:168:LEU:N	1:A:168:LEU:HD23	2.00	0.76
1:A:308:HIS:HB2	1:A:351:VAL:HA	1.68	0.76
1:A:565:LEU:HB3	1:A:594:ASP:HB3	1.67	0.76
1:A:108:ILE:HG12	1:A:527:LEU:HD13	1.68	0.76
1:A:409:ASP:O	1:A:411:SER:N	2.20	0.75
1:A:664:ASP:HB3	1:A:668:ARG:NH1	2.01	0.75
1:A:418:HIS:O	1:A:422:THR:HG23	1.87	0.75
1:A:126:CYS:HB2	1:A:271:GLN:HE22	1.51	0.74
1:A:324:ALA:HA	1:A:327:GLN:HE21	1.51	0.74
1:A:229:LYS:HE3	1:A:231:PHE:CE2	2.23	0.73
1:A:230:THR:CG2	1:A:231:PHE:N	2.51	0.73
1:A:325:LYS:O	1:A:329:SER:HB3	1.87	0.73
1:A:266:PRO:HB3	1:A:301:VAL:HG23	1.70	0.73
1:A:126:CYS:H	1:A:271:GLN:NE2	1.86	0.72
1:A:552:SER:HA	1:A:635:ARG:CZ	2.18	0.72
1:A:567:LEU:N	1:A:567:LEU:HD12	2.05	0.72
1:A:114:HIS:CD2	1:A:362:TYR:HB2	2.24	0.71
1:A:264:LYS:C	1:A:265:LEU:HD12	2.11	0.71
1:A:324:ALA:HB2	1:A:377:GLN:OE1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:HD11	1:A:532:TYR:CD2	2.27	0.70
1:A:147:PHE:O	1:A:160:ALA:N	2.24	0.70
1:A:178:SER:C	1:A:180:GLU:H	1.95	0.70
1:A:546:GLU:OE2	1:A:548:ARG:NE	2.25	0.70
1:A:515:GLU:HG3	1:A:515:GLU:O	1.91	0.69
1:A:64:ILE:N	1:A:64:ILE:HD12	2.08	0.69
1:A:161:ASP:OD1	1:A:192:LEU:HD22	1.93	0.68
1:A:661:THR:HG22	1:A:662:TRP:N	2.09	0.68
1:A:194:ASN:HD21	1:A:379:MET:CB	2.07	0.68
1:A:410:ARG:HG3	1:A:520:VAL:HG13	1.76	0.68
1:A:231:PHE:HD2	1:A:239:PRO:HA	1.59	0.68
1:A:567:LEU:CD1	1:A:619:ASP:HA	2.23	0.67
1:A:148:MET:O	1:A:222:VAL:HG22	1.95	0.67
1:A:576:PHE:CE1	1:A:623:VAL:HG13	2.29	0.67
1:A:657:ASN:HD22	1:A:657:ASN:N	1.90	0.67
1:A:243:ARG:HG3	1:A:243:ARG:O	1.95	0.67
1:A:616:VAL:HA	1:A:631:THR:O	1.96	0.66
1:A:178:SER:C	1:A:180:GLU:N	2.47	0.66
1:A:126:CYS:H	1:A:271:GLN:HE21	1.43	0.66
1:A:103:LEU:HD12	1:A:557:VAL:O	1.95	0.66
1:A:552:SER:HA	1:A:635:ARG:NH2	2.10	0.66
1:A:126:CYS:HB2	1:A:271:GLN:NE2	2.11	0.66
1:A:190:ALA:O	1:A:191:GLN:HB2	1.97	0.65
1:A:337:ARG:HH12	1:A:339:GLY:HA3	1.61	0.65
1:A:154:ASN:HD22	1:A:154:ASN:H	1.43	0.65
1:A:565:LEU:HD12	1:A:617:THR:HA	1.79	0.65
1:A:574:MET:HB2	1:A:575:PRO:HD3	1.77	0.64
1:A:669:TYR:HB3	1:A:670:PRO:HD2	1.79	0.64
1:A:607:THR:HG23	1:A:612:VAL:HB	1.79	0.64
1:A:339:GLY:O	1:A:343:GLU:HG2	1.97	0.63
1:A:147:PHE:HD1	1:A:200:LEU:HD13	1.64	0.63
1:A:513:VAL:HG23	1:A:513:VAL:O	1.97	0.63
1:A:323:SER:O	1:A:327:GLN:HG3	1.99	0.63
1:A:265:LEU:HD11	1:A:428:ALA:CB	2.27	0.63
1:A:565:LEU:HD11	1:A:604:TYR:OH	1.98	0.63
1:A:67:ARG:HG2	1:A:71:GLU:HG3	1.80	0.63
1:A:148:MET:CE	1:A:224:PHE:HB2	2.27	0.63
1:A:230:THR:HG23	1:A:231:PHE:H	1.64	0.63
1:A:168:LEU:O	1:A:172:MET:HG3	1.99	0.62
1:A:306:LYS:HD3	1:A:349:ASN:ND2	2.13	0.62
1:A:258:LEU:HG	1:A:263:GLY:HA2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:GLN:HA	1:A:547:GLN:OE1	1.99	0.62
1:A:198:GLN:O	1:A:201:ALA:N	2.32	0.62
1:A:395:SER:O	1:A:397:THR:HG23	1.99	0.62
1:A:596:SER:HB2	1:A:606:ARG:NH1	2.13	0.62
1:A:673:GLU:HG3	1:A:673:GLU:O	1.99	0.62
1:A:521:ILE:O	1:A:521:ILE:HG22	2.00	0.61
1:A:641:ILE:HD13	1:A:670:PRO:O	2.00	0.61
1:A:306:LYS:HD3	1:A:349:ASN:HD22	1.65	0.61
1:A:574:MET:O	1:A:576:PHE:N	2.33	0.61
1:A:116:ILE:HA	1:A:121:ILE:HB	1.82	0.61
1:A:357:GLY:O	1:A:361:LEU:HG	2.00	0.61
1:A:641:ILE:HD12	1:A:669:TYR:HB2	1.81	0.61
1:A:147:PHE:CD1	1:A:200:LEU:HD13	2.36	0.61
1:A:637:SER:C	1:A:639:ARG:H	2.04	0.61
1:A:219:SER:HB2	1:A:220:PRO:HD2	1.82	0.60
1:A:306:LYS:HZ1	1:A:519:ASN:HB3	1.66	0.60
1:A:287:ILE:HD12	1:A:402:ILE:CD1	2.31	0.60
1:A:65:VAL:HG11	1:A:536:GLU:OE2	2.02	0.60
1:A:71:GLU:O	1:A:75:LYS:HG3	2.01	0.60
1:A:114:HIS:CE1	1:A:358:ARG:NH2	2.70	0.60
1:A:668:ARG:HG3	1:A:668:ARG:HH11	1.67	0.60
1:A:538:THR:HB	1:A:552:SER:H	1.66	0.60
1:A:544:GLY:O	1:A:546:GLU:N	2.35	0.59
1:A:657:ASN:N	1:A:657:ASN:ND2	2.49	0.59
1:A:383:MET:HE1	1:A:390:CYS:HB3	1.84	0.59
1:A:172:MET:HG2	1:A:185:MET:HE3	1.84	0.59
1:A:277:ARG:O	1:A:279:GLU:N	2.36	0.59
1:A:362:TYR:CE1	1:A:366:VAL:HG21	2.38	0.59
1:A:319:LEU:O	1:A:319:LEU:HD12	2.02	0.59
1:A:297:ILE:HB	1:A:523:PRO:HD2	1.86	0.58
1:A:641:ILE:HG13	1:A:665:VAL:HG12	1.85	0.58
1:A:321:LEU:HD11	1:A:347:ILE:HD11	1.84	0.58
1:A:288:ARG:HH11	1:A:288:ARG:HG3	1.69	0.58
1:A:366:VAL:HG13	1:A:557:VAL:HG11	1.86	0.58
1:A:410:ARG:NH1	1:A:414:ASP:OD2	2.37	0.58
1:A:630:ALA:O	1:A:642:ARG:HD2	2.04	0.57
1:A:567:LEU:H	1:A:567:LEU:HD12	1.68	0.57
1:A:197:GLN:NE2	1:A:197:GLN:O	2.38	0.57
1:A:276:PHE:CD1	1:A:276:PHE:N	2.73	0.57
1:A:416:SER:O	1:A:420:ARG:HG3	2.05	0.57
1:A:231:PHE:CD2	1:A:239:PRO:HA	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:GLU:O	1:A:623:VAL:HG11	2.03	0.57
1:A:661:THR:HG22	1:A:663:ALA:H	1.68	0.57
1:A:580:LEU:O	1:A:584:LEU:HG	2.04	0.57
1:A:151:ASP:HA	1:A:218:LEU:HA	1.86	0.57
1:A:551:PHE:HB3	1:A:553:PHE:CE2	2.39	0.57
1:A:637:SER:O	1:A:639:ARG:HG3	2.05	0.57
1:A:560:PHE:CE1	1:A:592:LYS:HB2	2.39	0.56
1:A:637:SER:O	1:A:639:ARG:N	2.38	0.56
1:A:168:LEU:HD22	1:A:207:TYR:CD2	2.40	0.56
1:A:213:ILE:HD12	1:A:214:THR:CG2	2.25	0.56
1:A:661:THR:HG22	1:A:662:TRP:H	1.69	0.56
1:A:340:ASP:HA	1:A:343:GLU:HG2	1.88	0.56
1:A:184:GLU:O	1:A:188:VAL:HG23	2.05	0.56
1:A:409:ASP:OD1	1:A:409:ASP:O	2.24	0.56
1:A:145:ALA:CB	1:A:225:ASN:HA	2.32	0.56
1:A:211:SER:H	1:A:218:LEU:HD11	1.68	0.56
1:A:404:ILE:HG13	1:A:405:VAL:HG23	1.87	0.56
1:A:630:ALA:HB3	1:A:648:LEU:HD11	1.89	0.55
1:A:134:VAL:HG11	1:A:252:LEU:HD11	1.89	0.55
1:A:104:LYS:HG3	1:A:531:MET:HE1	1.88	0.55
1:A:311:PHE:CE2	1:A:315:ALA:HB2	2.41	0.55
1:A:362:TYR:O	1:A:366:VAL:HG23	2.07	0.55
1:A:580:LEU:HD22	1:A:618:ILE:HD11	1.88	0.55
1:A:570:ASN:H	1:A:570:ASN:ND2	2.03	0.55
2:A:1101:B4P:O3G	2:A:1101:B4P:H4F	2.06	0.55
1:A:336:MET:HE1	1:A:341:ALA:HA	1.88	0.55
1:A:91:SER:OG	1:A:282:PRO:HG2	2.07	0.55
1:A:340:ASP:HA	1:A:343:GLU:CG	2.37	0.55
1:A:206:ASN:C	1:A:208:ASN:H	2.10	0.55
1:A:337:ARG:NH1	1:A:339:GLY:HA3	2.21	0.55
1:A:542:ARG:NH2	1:A:636:ASP:O	2.40	0.54
1:A:558:ALA:O	1:A:559:PRO:C	2.43	0.54
1:A:633:ARG:HH21	1:A:638:MET:HG2	1.72	0.54
1:A:167:HIS:HB3	1:A:168:LEU:HD23	1.88	0.54
1:A:178:SER:O	1:A:180:GLU:N	2.40	0.54
1:A:164:LEU:O	1:A:164:LEU:HD22	2.08	0.54
1:A:228:PHE:CE2	1:A:278:ASN:HB2	2.42	0.54
1:A:574:MET:C	1:A:576:PHE:H	2.10	0.54
1:A:247:ALA:O	1:A:250:ILE:N	2.41	0.54
1:A:264:LYS:O	1:A:265:LEU:HD12	2.07	0.54
1:A:377:GLN:HG2	1:A:378:HIS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HG22	1:A:231:PHE:N	2.22	0.53
1:A:206:ASN:O	1:A:208:ASN:N	2.42	0.53
1:A:228:PHE:CZ	1:A:278:ASN:HB2	2.43	0.53
1:A:611:GLY:O	1:A:612:VAL:C	2.47	0.53
1:A:637:SER:C	1:A:639:ARG:N	2.62	0.53
1:A:153:LYS:HG2	1:A:216:ASN:HB3	1.91	0.53
1:A:153:LYS:CG	1:A:216:ASN:HB3	2.38	0.53
1:A:302:ASP:HB3	1:A:305:GLU:HB2	1.90	0.53
1:A:294:MET:HB2	1:A:525:PHE:O	2.09	0.53
1:A:322:TYR:CE2	1:A:327:GLN:HG2	2.44	0.53
1:A:157:CYS:O	1:A:158:PHE:CG	2.62	0.52
1:A:292:PHE:HE2	1:A:294:MET:HE3	1.74	0.52
1:A:192:LEU:HD23	1:A:192:LEU:O	2.09	0.52
1:A:336:MET:CE	1:A:341:ALA:HA	2.40	0.52
1:A:194:ASN:HD22	1:A:381:ASN:ND2	2.07	0.52
1:A:668:ARG:HB2	1:A:669:TYR:CD1	2.45	0.52
1:A:153:LYS:HG3	1:A:216:ASN:ND2	2.25	0.52
1:A:228:PHE:O	1:A:241:TYR:HD1	1.93	0.52
1:A:148:MET:HA	1:A:158:PHE:O	2.10	0.52
1:A:389:ASP:O	1:A:390:CYS:HB2	2.10	0.52
1:A:565:LEU:HB3	1:A:594:ASP:CB	2.37	0.52
1:A:265:LEU:HD11	1:A:428:ALA:HB1	1.91	0.52
1:A:318:HIS:CE1	1:A:337:ARG:HB2	2.45	0.52
1:A:322:TYR:HD2	1:A:376:ARG:HG3	1.75	0.52
1:A:113:GLN:O	1:A:115:PHE:N	2.43	0.52
1:A:151:ASP:HB3	1:A:218:LEU:HD12	1.91	0.52
1:A:669:TYR:CD1	1:A:669:TYR:N	2.78	0.51
1:A:351:VAL:HG12	1:A:352:LEU:N	2.25	0.51
1:A:211:SER:N	1:A:218:LEU:CD1	2.69	0.51
1:A:317:LEU:HD11	1:A:361:LEU:HD21	1.91	0.51
1:A:569:GLN:HG3	1:A:569:GLN:O	2.11	0.51
1:A:355:PHE:O	1:A:359:ILE:HG13	2.11	0.51
1:A:567:LEU:CD1	1:A:567:LEU:N	2.73	0.51
1:A:124:ILE:O	1:A:271:GLN:HG3	2.11	0.51
1:A:209:VAL:HG12	1:A:218:LEU:CD2	2.39	0.50
1:A:138:SER:O	1:A:385:HIS:HE1	1.93	0.50
1:A:567:LEU:H	1:A:567:LEU:CD1	2.24	0.50
1:A:206:ASN:C	1:A:208:ASN:N	2.64	0.50
1:A:250:ILE:HG21	1:A:298:GLU:HB2	1.92	0.50
1:A:520:VAL:O	1:A:521:ILE:HD12	2.11	0.50
1:A:112:ARG:HG2	1:A:112:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HD12	1:A:298:GLU:HG2	1.93	0.50
1:A:211:SER:N	1:A:218:LEU:HD11	2.25	0.50
1:A:134:VAL:CG1	1:A:252:LEU:HD11	2.41	0.50
1:A:288:ARG:CG	1:A:288:ARG:HH11	2.25	0.50
1:A:306:LYS:HZ1	1:A:519:ASN:CB	2.24	0.50
1:A:554:PRO:O	1:A:556:VAL:N	2.45	0.50
1:A:172:MET:HG2	1:A:185:MET:CE	2.42	0.50
1:A:83:ALA:O	1:A:84:PHE:C	2.49	0.50
1:A:335:LYS:O	1:A:335:LYS:HG2	2.12	0.50
1:A:580:LEU:CD2	1:A:618:ILE:HD11	2.42	0.50
1:A:74:LEU:CD1	1:A:80:TYR:HE1	2.22	0.50
1:A:565:LEU:HD12	1:A:565:LEU:O	2.11	0.50
1:A:166:ALA:O	1:A:170:LYS:HE2	2.12	0.49
1:A:637:SER:HB2	1:A:639:ARG:HG3	1.94	0.49
1:A:201:ALA:HA	1:A:221:PRO:CG	2.38	0.49
1:A:151:ASP:HB2	1:A:216:ASN:HB2	1.93	0.49
1:A:562:CYS:SG	1:A:563:SER:N	2.85	0.49
1:A:314:VAL:HG21	1:A:354:TYR:HA	1.94	0.49
1:A:299:HIS:CD2	1:A:355:PHE:HZ	2.31	0.49
1:A:65:VAL:HG22	1:A:66:ASP:N	2.27	0.49
1:A:152:VAL:HG12	1:A:152:VAL:O	2.12	0.49
1:A:599:SER:O	1:A:603:ARG:HG2	2.12	0.49
1:A:623:VAL:HG12	1:A:623:VAL:O	2.13	0.49
1:A:104:LYS:HG3	1:A:531:MET:CE	2.43	0.49
1:A:317:LEU:CD1	1:A:361:LEU:HD21	2.42	0.49
1:A:146:ASP:HB3	1:A:159:ARG:HG3	1.95	0.49
1:A:311:PHE:CD2	1:A:311:PHE:C	2.86	0.49
1:A:160:ALA:O	1:A:161:ASP:C	2.50	0.49
1:A:178:SER:HB2	1:A:180:GLU:HB2	1.94	0.49
1:A:148:MET:HE2	1:A:224:PHE:HB2	1.95	0.49
1:A:411:SER:OG	1:A:412:CYS:N	2.46	0.49
1:A:552:SER:CA	1:A:635:ARG:NH2	2.75	0.49
1:A:211:SER:CA	1:A:218:LEU:HD11	2.42	0.49
1:A:514:GLU:HG2	1:A:515:GLU:N	2.28	0.49
1:A:403:GLU:OE2	2:A:1101:B4P:O2G	2.31	0.48
1:A:281:SER:O	1:A:283:ARG:HG3	2.13	0.48
1:A:587:HIS:O	1:A:653:GLN:NE2	2.46	0.48
2:A:1101:B4P:O2B	2:A:1101:B4P:H52A	2.13	0.48
1:A:145:ALA:HB1	1:A:224:PHE:C	2.31	0.48
1:A:574:MET:C	1:A:576:PHE:N	2.67	0.48
1:A:599:SER:O	1:A:600:ILE:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ASP:O	1:A:625:LYS:HB2	2.13	0.48
1:A:112:ARG:HG2	1:A:112:ARG:NH1	2.28	0.48
1:A:366:VAL:O	1:A:366:VAL:HG12	2.12	0.48
1:A:395:SER:HB2	1:A:533:THR:HG21	1.94	0.48
1:A:302:ASP:OD2	1:A:430:LYS:HD2	2.12	0.48
1:A:322:TYR:CD1	1:A:333:ALA:HB2	2.48	0.48
1:A:311:PHE:HE2	1:A:315:ALA:HB2	1.77	0.48
1:A:375:PHE:HA	1:A:392:ASP:O	2.14	0.48
1:A:368:ILE:CD1	1:A:533:THR:HB	2.44	0.48
1:A:329:SER:O	1:A:329:SER:OG	2.27	0.47
1:A:420:ARG:O	1:A:422:THR:N	2.47	0.47
1:A:168:LEU:HD23	1:A:168:LEU:H	1.77	0.47
1:A:177:CYS:SG	1:A:182:LYS:HB2	2.54	0.47
1:A:573:PHE:O	1:A:576:PHE:HB2	2.14	0.47
1:A:620:PHE:HD1	1:A:620:PHE:H	1.60	0.47
1:A:522:GLU:HA	1:A:523:PRO:HD3	1.77	0.47
1:A:247:ALA:O	1:A:248:GLN:C	2.52	0.47
1:A:193:ASP:CB	1:A:382:GLU:HG3	2.39	0.47
1:A:620:PHE:HB3	1:A:624:ASN:ND2	2.22	0.47
1:A:106:ASN:HB3	1:A:557:VAL:HA	1.97	0.47
1:A:194:ASN:HB3	1:A:381:ASN:HD21	1.80	0.47
1:A:226:LEU:O	1:A:278:ASN:HB3	2.15	0.47
1:A:162:HIS:HE1	1:A:288:ARG:NH1	2.13	0.46
1:A:114:HIS:HD2	1:A:115:PHE:CZ	2.33	0.46
1:A:320:TYR:HA	1:A:334:ARG:O	2.15	0.46
1:A:311:PHE:HD1	1:A:350:THR:O	1.99	0.46
1:A:74:LEU:HD13	1:A:80:TYR:CE1	2.38	0.46
1:A:544:GLY:C	1:A:546:GLU:N	2.69	0.46
1:A:339:GLY:O	1:A:343:GLU:OE2	2.33	0.46
1:A:85:ALA:C	1:A:87:TYR:H	2.17	0.46
1:A:172:MET:HB3	1:A:182:LYS:HG3	1.96	0.46
1:A:147:PHE:HA	1:A:222:VAL:O	2.16	0.46
1:A:617:THR:CB	1:A:631:THR:HB	2.17	0.46
1:A:325:LYS:C	1:A:327:GLN:H	2.17	0.46
1:A:389:ASP:O	1:A:390:CYS:CB	2.64	0.46
1:A:570:ASN:N	1:A:570:ASN:ND2	2.63	0.46
1:A:168:LEU:C	1:A:170:LYS:H	2.19	0.46
1:A:214:THR:HG23	1:A:216:ASN:OD1	2.16	0.46
1:A:229:LYS:HD3	1:A:230:THR:N	2.31	0.46
1:A:211:SER:HB3	1:A:216:ASN:H	1.81	0.45
1:A:311:PHE:CD1	1:A:350:THR:HB	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASP:OD2	1:A:69:LYS:CB	2.64	0.45
1:A:608:ASP:OD2	1:A:633:ARG:NH2	2.48	0.45
1:A:132:GLU:HB3	1:A:133:PRO:CD	2.41	0.45
1:A:411:SER:O	1:A:519:ASN:HA	2.16	0.45
1:A:140:HIS:C	1:A:142:ASP:N	2.70	0.45
1:A:210:LYS:O	1:A:211:SER:C	2.55	0.45
1:A:367:GLY:O	1:A:368:ILE:C	2.54	0.45
1:A:132:GLU:H	1:A:240:GLY:HA2	1.81	0.45
1:A:526:GLY:O	1:A:530:ILE:HG13	2.16	0.45
1:A:626:THR:HA	1:A:627:PRO:C	2.37	0.45
1:A:114:HIS:O	1:A:358:ARG:NH1	2.50	0.45
1:A:386:TYR:CZ	1:A:410:ARG:NH2	2.85	0.45
1:A:66:ASP:OD2	1:A:69:LYS:HB3	2.17	0.45
1:A:85:ALA:O	1:A:87:TYR:N	2.48	0.45
1:A:247:ALA:O	1:A:249:GLY:N	2.49	0.44
1:A:565:LEU:HD11	1:A:604:TYR:CZ	2.52	0.44
1:A:229:LYS:NZ	1:A:239:PRO:HB2	2.32	0.44
1:A:144:PHE:HZ	1:A:277:ARG:CD	2.30	0.44
1:A:255:LYS:HD3	1:A:255:LYS:HA	1.82	0.44
1:A:377:GLN:HG3	1:A:390:CYS:O	2.17	0.44
1:A:651:ILE:HG22	1:A:655:LEU:HD12	2.00	0.44
1:A:661:THR:CG2	1:A:662:TRP:N	2.76	0.44
1:A:159:ARG:HH11	1:A:162:HIS:CE1	2.36	0.44
1:A:381:ASN:HD22	1:A:381:ASN:H	1.65	0.44
1:A:582:GLU:O	1:A:585:THR:HB	2.17	0.44
1:A:138:SER:O	1:A:385:HIS:CE1	2.71	0.44
1:A:150:LYS:HB2	1:A:155:GLY:O	2.18	0.44
1:A:191:GLN:HB2	1:A:191:GLN:HE21	1.68	0.43
1:A:284:SER:HA	1:A:399:TYR:HE2	1.83	0.43
1:A:597:SER:O	1:A:606:ARG:NH2	2.48	0.43
1:A:113:GLN:HA	1:A:113:GLN:OE1	2.17	0.43
1:A:277:ARG:NH2	2:A:1101:B4P:O1D	2.50	0.43
1:A:211:SER:HB2	1:A:218:LEU:HD11	2.00	0.43
1:A:620:PHE:N	1:A:620:PHE:CD1	2.87	0.43
1:A:147:PHE:HE2	1:A:223:SER:OG	2.00	0.43
1:A:144:PHE:O	1:A:145:ALA:HB2	2.19	0.43
1:A:164:LEU:CD2	1:A:168:LEU:HD21	2.49	0.43
1:A:363:LEU:HD11	1:A:405:VAL:HG21	1.99	0.43
1:A:525:PHE:N	1:A:525:PHE:CD1	2.85	0.43
1:A:202:ASP:O	1:A:204:PHE:N	2.52	0.43
1:A:247:ALA:HB2	1:A:298:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HG2	1:A:256:ARG:H	1.65	0.43
1:A:561:LYS:HD3	1:A:656:ALA:HB1	2.00	0.43
1:A:86:ILE:HG13	1:A:87:TYR:HD1	1.83	0.43
1:A:181:LYS:HE3	1:A:185:MET:SD	2.59	0.43
1:A:316:ASP:O	1:A:317:LEU:C	2.57	0.43
1:A:382:GLU:HG2	1:A:382:GLU:O	2.19	0.43
1:A:144:PHE:CZ	1:A:277:ARG:HD3	2.54	0.43
1:A:322:TYR:O	1:A:323:SER:O	2.37	0.43
1:A:190:ALA:O	1:A:191:GLN:NE2	2.51	0.42
1:A:211:SER:O	1:A:215:GLY:HA2	2.18	0.42
1:A:288:ARG:CG	1:A:288:ARG:NH1	2.80	0.42
1:A:302:ASP:HB3	1:A:305:GLU:CG	2.49	0.42
1:A:574:MET:CB	1:A:575:PRO:HD3	2.44	0.42
1:A:578:LYS:O	1:A:579:GLU:C	2.56	0.42
1:A:302:ASP:HB3	1:A:305:GLU:CB	2.48	0.42
1:A:369:SER:O	1:A:370:PRO:C	2.58	0.42
1:A:410:ARG:O	1:A:411:SER:C	2.58	0.42
1:A:565:LEU:CB	1:A:594:ASP:HB3	2.45	0.42
1:A:430:LYS:O	1:A:513:VAL:HA	2.20	0.42
1:A:308:HIS:HA	1:A:309:PRO:HD3	1.61	0.42
1:A:377:GLN:NE2	1:A:389:ASP:OD1	2.53	0.42
1:A:377:GLN:N	1:A:391:TRP:CE3	2.87	0.42
1:A:414:ASP:O	1:A:418:HIS:HD2	2.03	0.42
1:A:513:VAL:CG2	1:A:513:VAL:O	2.66	0.42
1:A:141:VAL:N	1:A:227:MET:HE1	2.34	0.42
1:A:248:GLN:O	1:A:252:LEU:HG	2.20	0.42
1:A:339:GLY:O	1:A:343:GLU:CG	2.67	0.42
1:A:668:ARG:NH1	1:A:668:ARG:HG3	2.32	0.42
1:A:306:LYS:O	1:A:349:ASN:HB2	2.20	0.42
1:A:396:LYS:HG2	1:A:401:TRP:CE2	2.55	0.42
1:A:564:VAL:HG11	1:A:580:LEU:HD23	2.01	0.42
1:A:594:ASP:OD1	1:A:603:ARG:HB3	2.19	0.42
1:A:374:ARG:HG2	1:A:401:TRP:CE3	2.55	0.42
1:A:154:ASN:HD22	1:A:154:ASN:N	2.08	0.41
1:A:554:PRO:C	1:A:556:VAL:N	2.73	0.41
1:A:219:SER:HB2	1:A:220:PRO:CD	2.46	0.41
1:A:279:GLU:OE2	1:A:288:ARG:NE	2.52	0.41
1:A:298:GLU:HA	1:A:298:GLU:OE1	2.18	0.41
1:A:311:PHE:CD2	1:A:311:PHE:O	2.74	0.41
1:A:104:LYS:CG	1:A:531:MET:HE1	2.49	0.41
1:A:80:TYR:HA	1:A:95:ASP:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ALA:HA	1:A:586:ARG:NH1	2.35	0.41
1:A:372:LYS:HB2	1:A:537:HIS:CE1	2.56	0.41
1:A:122:LEU:HD21	1:A:260:PHE:HD2	1.86	0.41
1:A:111:TRP:HB2	1:A:362:TYR:OH	2.21	0.41
1:A:151:ASP:C	1:A:153:LYS:H	2.24	0.41
1:A:379:MET:H	1:A:382:GLU:HB3	1.85	0.41
1:A:70:MET:HG3	1:A:539:PHE:CD2	2.55	0.41
1:A:561:LYS:HD3	1:A:656:ALA:CB	2.51	0.41
1:A:65:VAL:CG2	1:A:66:ASP:N	2.84	0.41
1:A:337:ARG:NH1	1:A:339:GLY:CA	2.84	0.41
1:A:633:ARG:NH2	1:A:638:MET:HG2	2.36	0.41
1:A:168:LEU:N	1:A:168:LEU:CD2	2.72	0.41
1:A:377:GLN:HB2	1:A:391:TRP:CE3	2.55	0.41
1:A:111:TRP:NE1	1:A:525:PHE:CD2	2.89	0.41
1:A:577:VAL:O	1:A:578:LYS:C	2.59	0.41
1:A:409:ASP:CG	1:A:521:ILE:HD11	2.41	0.41
1:A:599:SER:O	1:A:602:ARG:N	2.54	0.40
1:A:377:GLN:HB2	1:A:391:TRP:CZ3	2.57	0.40
1:A:560:PHE:CE2	1:A:592:LYS:HD2	2.56	0.40
1:A:621:ASP:HA	1:A:625:LYS:HD3	2.03	0.40
1:A:149:VAL:O	1:A:150:LYS:HB3	2.21	0.40
1:A:267:PHE:O	1:A:267:PHE:CG	2.75	0.40
1:A:374:ARG:HG2	1:A:401:TRP:CZ3	2.57	0.40
1:A:386:TYR:CE2	1:A:410:ARG:NH2	2.90	0.40
1:A:306:LYS:NZ	1:A:519:ASN:CB	2.85	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	526/693 (76%)	388 (74%)	84 (16%)	54 (10%)	0	3

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	A	114	HIS
1	A	156	GLU
1	A	191	GLN
1	A	206	ASN
1	A	215	GLY
1	A	278	ASN
1	A	306	LYS
1	A	323	SER
1	A	330	GLY
1	A	336	MET
1	A	348	ASN
1	A	410	ARG
1	A	411	SER
1	A	413	TYR
1	A	420	ARG
1	A	421	ALA
1	A	545	ASP
1	A	638	MET
1	A	660	ILE
1	A	152	VAL
1	A	161	ASP
1	A	207	TYR
1	A	208	ASN
1	A	211	SER
1	A	219	SER
1	A	344	GLN
1	A	380	GLU
1	A	561	LYS
1	A	635	ARG
1	A	150	LYS
1	A	182	LYS
1	A	203	LEU
1	A	390	CYS
1	A	537	HIS
1	A	555	ALA
1	A	612	VAL
1	A	199	GLU
1	A	317	LEU
1	A	575	PRO
1	A	578	LYS
1	A	68	ALA

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	282	PRO
1	A	346	VAL
1	A	523	PRO
1	A	613	ALA
1	A	672	PHE
1	A	248	GLN
1	A	309	PRO
1	A	600	ILE
1	A	236	GLY
1	A	243	ARG
1	A	98	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	460/600 (77%)	410 (89%)	50 (11%)	6	23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	A	72	ASP
1	A	78	PHE
1	A	133	PRO
1	A	154	ASN
1	A	163	LEU
1	A	164	LEU
1	A	168	LEU
1	A	177	CYS
1	A	183	SER
1	A	184	GLU
1	A	191	GLN
1	A	193	ASP
1	A	204	PHE

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Mol	Chain	Res	Type
1	A	217	ASP
1	A	237	ASN
1	A	245	GLU
1	A	259	GLU
1	A	264	LYS
1	A	276	PHE
1	A	281	SER
1	A	284	SER
1	A	288	ARG
1	A	294	MET
1	A	301	VAL
1	A	307	ASP
1	A	313	ASN
1	A	319	LEU
1	A	329	SER
1	A	340	ASP
1	A	348	ASN
1	A	381	ASN
1	A	386	TYR
1	A	422	THR
1	A	517	VAL
1	A	542	ARG
1	A	545	ASP
1	A	556	VAL
1	A	557	VAL
1	A	565	LEU
1	A	570	ASN
1	A	572	GLU
1	A	577	VAL
1	A	595	ASP
1	A	600	ILE
1	A	607	THR
1	A	641	ILE
1	A	655	LEU
1	A	657	ASN
1	A	660	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	114	HIS

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Mol	Chain	Res	Type
1	A	154	ASN
1	A	162	HIS
1	A	169	GLN
1	A	194	ASN
1	A	197	GLN
1	A	206	ASN
1	A	261	ASN
1	A	271	GLN
1	A	299	HIS
1	A	313	ASN
1	A	327	GLN
1	A	348	ASN
1	A	381	ASN
1	A	519	ASN
1	A	570	ASN
1	A	624	ASN
1	A	640	GLN
1	A	657	ASN
1	A	659	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	B4P	A	1101	-	46,58,58	1.24	6 (13%)	49,91,91	1.47	7 (14%)

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	B4P	A	1101	-	4/4/12/12	5/30/70/70	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	B4P	PD-O1D	2.99	1.61	1.50
2	A	1101	B4P	PG-O1G	2.98	1.61	1.50
2	A	1101	B4P	PA-O1A	2.97	1.61	1.50
2	A	1101	B4P	PB-O1B	2.97	1.61	1.50
2	A	1101	B4P	O4F-C1F	2.37	1.44	1.41
2	A	1101	B4P	O4E-C1E	2.28	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	B4P	N3A-C2A-N1A	-4.46	121.70	128.68
2	A	1101	B4P	N3B-C2B-N1B	-4.39	121.81	128.68
2	A	1101	B4P	PD-O3G-PG	-3.08	122.27	132.83
2	A	1101	B4P	C2F-C3F-C4F	-2.72	97.35	102.64
2	A	1101	B4P	PG-O3B-PB	-2.68	123.64	132.83
2	A	1101	B4P	O4E-C1E-C2E	-2.44	103.36	106.93
2	A	1101	B4P	PB-O3A-PA	-2.07	125.72	132.83

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1101	B4P	C4E
2	A	1101	B4P	C3F
2	A	1101	B4P	C3E
2	A	1101	B4P	C4F

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	B4P	C4F-C5F-O5F-PD
2	A	1101	B4P	O4E-C4E-C5E-O5E
2	A	1101	B4P	PG-O3B-PB-O2B
2	A	1101	B4P	PB-O3A-PA-O5E
2	A	1101	B4P	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	B4P	4	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 B4P A 1101

Bond lengths

Bond angles

Torsions

Rings
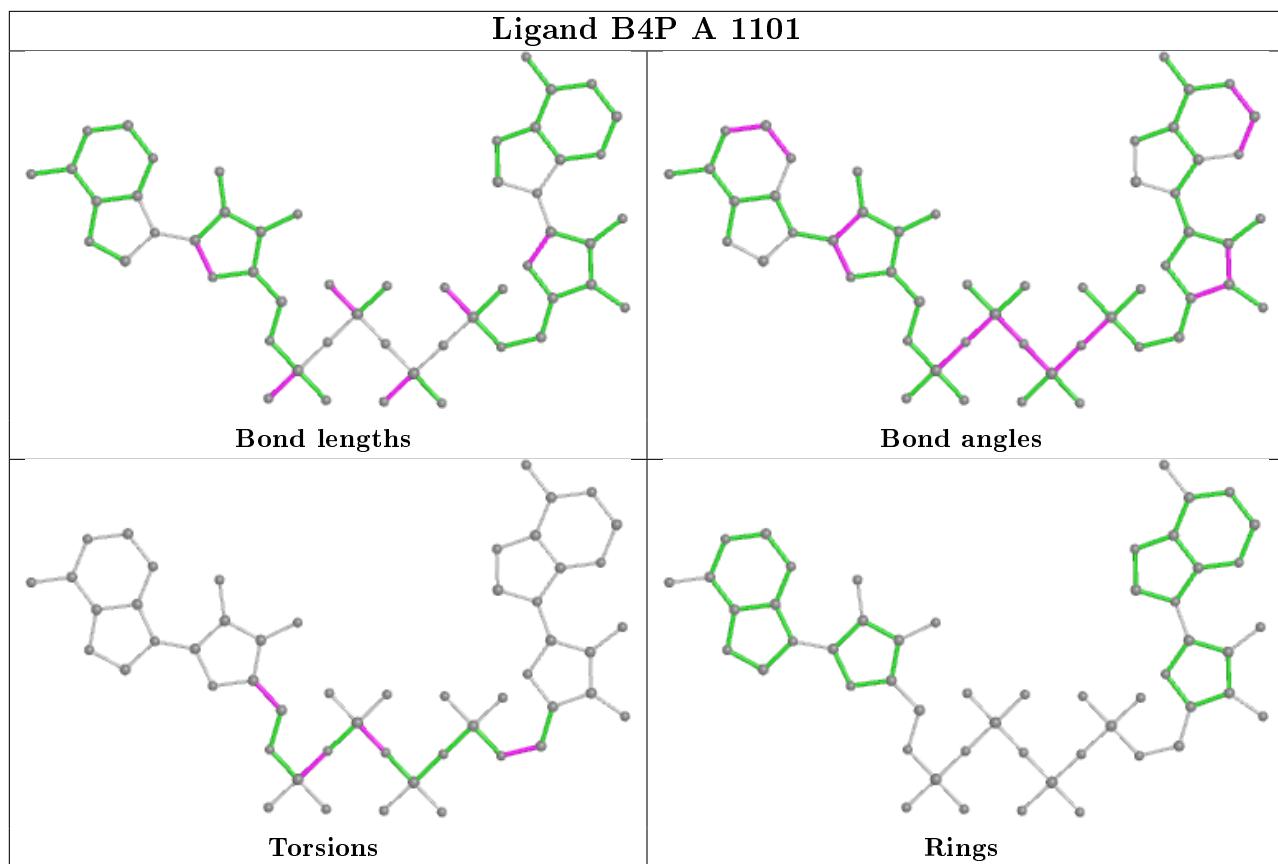
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	530/693 (76%)	0.70	62 (11%)	4	5	124, 170, 199, 200	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	LYS	5.2
1	A	512	TYR	5.1
1	A	207	TYR	4.7
1	A	179	VAL	4.2
1	A	274	ASN	3.9
1	A	662	TRP	3.9
1	A	427	VAL	3.9
1	A	673	GLU	3.8
1	A	212	PRO	3.7
1	A	618	ILE	3.6
1	A	173	SER	3.6
1	A	314	VAL	3.6
1	A	549	THR	3.6
1	A	513	VAL	3.5
1	A	209	VAL	3.5
1	A	672	PHE	3.4
1	A	125	ASP	3.4
1	A	514	GLU	3.4
1	A	293	THR	3.3
1	A	344	GLN	3.2
1	A	346	VAL	3.2
1	A	273	GLY	3.2
1	A	174	ASP	3.2
1	A	336	MET	3.1
1	A	541	VAL	3.1
1	A	338	LEU	3.1
1	A	126	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	573	PHE	3.0
1	A	429	GLU	3.0
1	A	545	ASP	2.9
1	A	426	LEU	2.9
1	A	317	LEU	2.9
1	A	632	LEU	2.9
1	A	518	PRO	2.8
1	A	428	ALA	2.8
1	A	548	ARG	2.8
1	A	616	VAL	2.7
1	A	158	PHE	2.7
1	A	347	ILE	2.6
1	A	516	VAL	2.6
1	A	312	GLN	2.5
1	A	151	ASP	2.3
1	A	213	ILE	2.3
1	A	580	LEU	2.3
1	A	321	LEU	2.3
1	A	638	MET	2.3
1	A	311	PHE	2.3
1	A	625	LYS	2.3
1	A	576	PHE	2.2
1	A	619	ASP	2.2
1	A	156	GLU	2.2
1	A	551	PHE	2.2
1	A	640	GLN	2.2
1	A	300	PHE	2.1
1	A	149	VAL	2.1
1	A	360	TYR	2.1
1	A	575	PRO	2.1
1	A	652	VAL	2.0
1	A	280	ILE	2.0
1	A	617	THR	2.0
1	A	566	PRO	2.0
1	A	127	THR	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 carbohydrates 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	B4P	A	1101	53/53	0.82	0.29	176,198,200,200	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 B4P A 1101:

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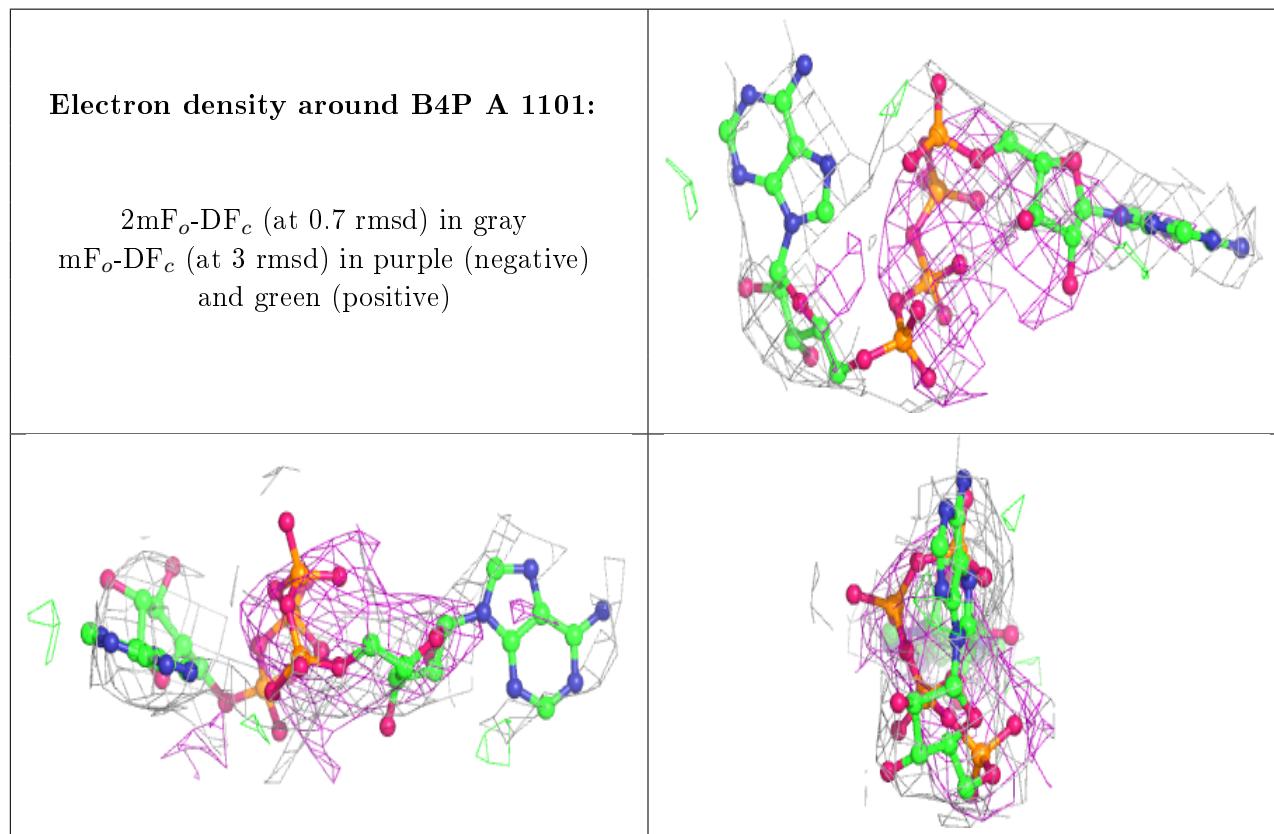
6.5 Other polymers (i)

There are no such residues in this entry.