



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 04:44 AM EDT

PDB ID : 1K6M  
Title : Crystal Structure of Human Liver 6-Phosphofructo-2-Kinase/Fructose-2,6-Bi  
sphosphatase  
Authors : Lee, Y.H.; Li, Y.; Uyeda, K.; Hasemann, C.A.  
Deposited on : 2001-10-16  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

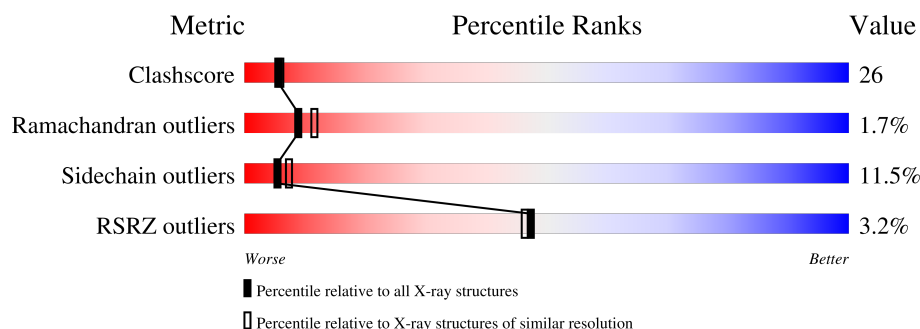
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	432	<div> <div>3%</div> <div>57%</div> <div>34%</div> <div>8%</div> </div>
1	B	432	<div> <div>3%</div> <div>58%</div> <div>33%</div> <div>7%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7545 atoms, of which 12 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.

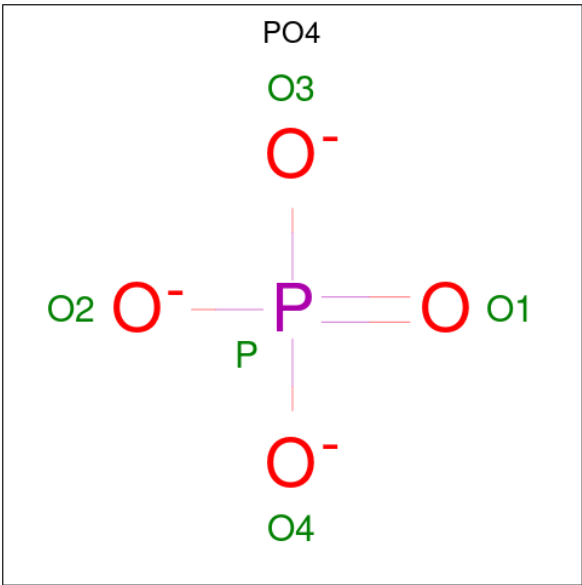
- Molecule 1 is a protein called 6-phosphofructo-2-kinase/fructose-2,6-biphosphatase 2-phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3527	2237	605	666	19			
1	B	432	Total	C	N	O	S	0	0	0
			3527	2237	605	666	19			

There are 8 discrepancies between the modelled and reference sequences:

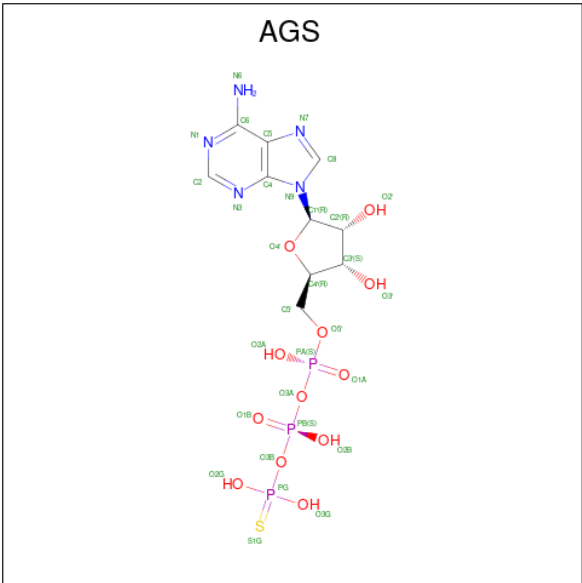
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	PHE	TRP	engineered mutation	UNP P16118
A	301	PHE	TRP	engineered mutation	UNP P16118
A	322	PHE	TRP	engineered mutation	UNP P16118
A	409	GLU	ASP	engineered mutation	UNP P16118
B	67	PHE	TRP	engineered mutation	UNP P16118
B	301	PHE	TRP	engineered mutation	UNP P16118
B	322	PHE	TRP	engineered mutation	UNP P16118
B	409	GLU	ASP	engineered mutation	UNP P16118

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			37	10	6	5	12	3	1		
3	B	1	Total	C	H	N	O	P	S	0	0
			37	10	6	5	12	3	1		

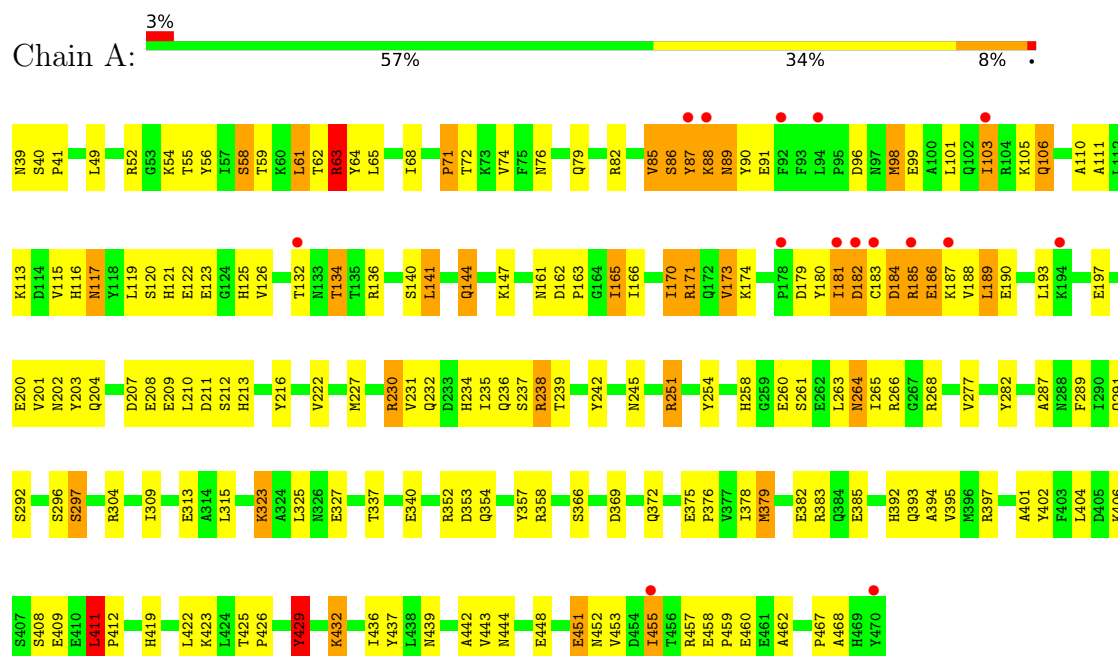
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	196	Total	O	0	0
			196	196		
4	B	201	Total	O	0	0
			201	201		

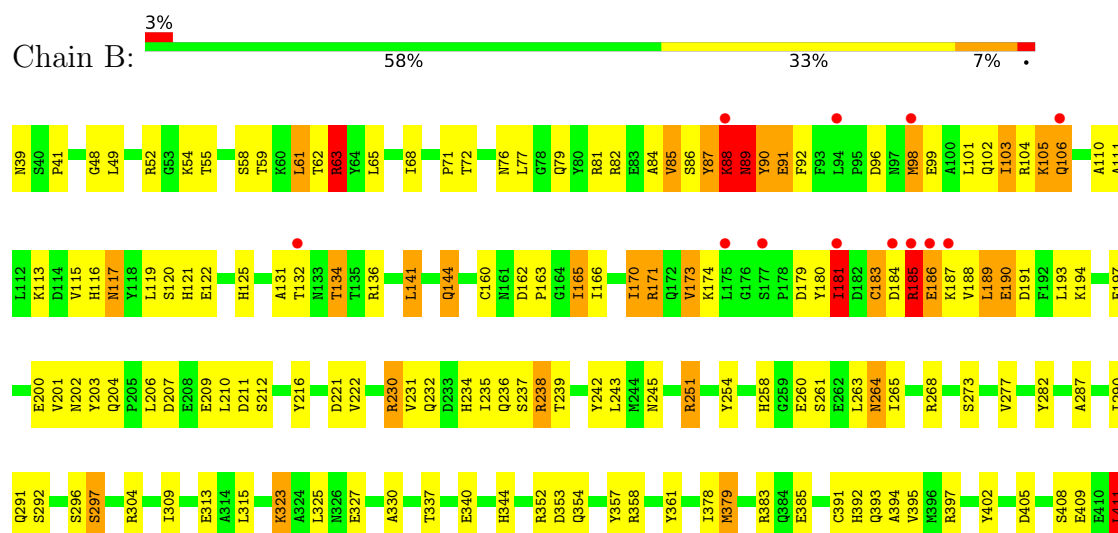
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 6-phosphofructo-2-kinase/fructose-2,6-biphosphatase 2-phosphatase



- Molecule 1: 6-phosphofructo-2-kinase/fructose-2,6-biphosphatase 2-phosphatase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.98Å 185.33Å 89.67Å 90.00° 90.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	10.0 (30.00-2.40) 40.7 (29.89-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.217 , 0.257 0.214 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, AGS

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	0.57	0/3601	0.80	6/4870 (0.1%)
1	B	0.57	0/3601	0.79	4/4870 (0.1%)
All	All	0.57	0/7202	0.79	10/9740 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	LYS	N-CA-C	7.76	131.95	111.00
1	A	63	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	87	TYR	N-CA-C	7.10	130.18	111.00
1	B	63	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	411	LEU	CA-CB-CG	6.80	130.94	115.30
1	B	411	LEU	CA-CB-CG	6.62	130.53	115.30
1	A	63	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	87	TYR	N-CA-C	5.69	126.35	111.00
1	B	63	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	89	ASN	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3527	0	3482	181	0
1	B	3527	0	3482	186	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
3	A	31	6	12	4	0
3	B	31	6	12	3	0
4	A	196	0	0	50	1
4	B	201	0	0	31	1
All	All	7533	12	6988	363	1

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 (363) 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:126:VAL:HG23	4:A:656:HOH:O	1.52	1.09
1:B:409:GLU:HG3	4:B:688:HOH:O	1.52	1.07
1:A:58:SER:HB3	4:A:682:HOH:O	1.56	1.06
1:A:238:ARG:HE	1:A:238:ARG:HA	1.26	1.00
1:A:378:ILE:HG22	4:A:671:HOH:O	1.60	0.99
1:A:63:ARG:HA	4:A:709:HOH:O	1.60	0.99
1:A:125:HIS:HB3	4:A:656:HOH:O	1.61	0.99
1:A:451:GLU:HG2	4:A:661:HOH:O	1.62	0.99
1:B:238:ARG:HE	1:B:238:ARG:HA	1.28	0.98
1:A:63:ARG:HH11	1:A:63:ARG:HB2	1.26	0.97
1:B:189:LEU:HG	4:B:778:HOH:O	1.64	0.97
1:A:63:ARG:HH11	1:A:63:ARG:CB	1.77	0.96
1:A:74:VAL:HG11	4:A:682:HOH:O	1.67	0.95
1:B:63:ARG:HB2	1:B:63:ARG:HH11	1.32	0.94
1:A:208:GLU:HB3	4:A:743:HOH:O	1.68	0.93
1:B:206:LEU:HG	4:B:714:HOH:O	1.70	0.92
1:A:409:GLU:HG3	4:A:623:HOH:O	1.70	0.90
1:B:63:ARG:HH11	1:B:63:ARG:CB	1.85	0.90
1:A:201:VAL:HG12	1:A:202:ASN:OD1	1.76	0.85
1:A:162:ASP:HB3	1:A:165:ILE:HG13	1.56	0.85
1:B:201:VAL:HG12	1:B:202:ASN:OD1	1.76	0.85
1:A:406:LYS:HG2	4:A:672:HOH:O	1.76	0.83
1:A:85:VAL:HG12	1:A:86:SER:H	1.43	0.83
1:B:63:ARG:HB2	1:B:63:ARG:NH1	1.94	0.83
1:B:238:ARG:HA	1:B:238:ARG:NE	1.92	0.83
1:A:63:ARG:CB	1:A:63:ARG:NH1	2.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HB2	1:A:63:ARG:NH1	1.94	0.82
1:B:162:ASP:HB3	1:B:165:ILE:HG13	1.61	0.82
1:A:238:ARG:HA	1:A:238:ARG:NE	1.89	0.81
1:A:63:ARG:NH2	1:A:402:TYR:O	2.12	0.81
1:B:160:CYS:HB3	4:B:634:HOH:O	1.79	0.81
1:A:426:PRO:HD2	4:A:703:HOH:O	1.81	0.81
1:A:87:TYR:HE2	1:A:181:ILE:HG13	1.47	0.80
1:B:63:ARG:CB	1:B:63:ARG:NH1	2.45	0.79
1:B:136:ARG:HH12	1:B:210:LEU:HB3	1.47	0.79
1:A:136:ARG:HH12	1:A:210:LEU:HB3	1.48	0.77
1:A:82:ARG:HD3	1:A:179:ASP:OD1	1.84	0.77
1:B:39:ASN:HB2	4:B:733:HOH:O	1.84	0.76
1:B:189:LEU:CD1	1:B:193:LEU:HG	2.16	0.76
1:B:160:CYS:SG	4:B:667:HOH:O	2.43	0.75
1:B:304:ARG:HG3	1:B:323:LYS:HA	1.67	0.75
1:A:304:ARG:HG3	1:A:323:LYS:HA	1.67	0.75
1:B:245:ASN:OD1	1:B:383:ARG:HD3	1.88	0.74
1:A:61:LEU:HD11	1:A:239:THR:HG23	1.70	0.73
1:B:85:VAL:HG13	1:B:86:SER:N	2.00	0.73
1:A:189:LEU:CD1	1:A:193:LEU:HG	2.19	0.73
1:A:245:ASN:OD1	1:A:383:ARG:HD3	1.87	0.73
1:B:203:TYR:HB3	4:B:798:HOH:O	1.87	0.73
1:B:415:LYS:HE3	4:B:699:HOH:O	1.88	0.73
1:A:59:THR:O	1:A:63:ARG:HG2	1.89	0.72
1:B:76:ASN:HB3	1:B:79:GLN:HG3	1.72	0.72
1:B:448:GLU:HG3	4:B:612:HOH:O	1.89	0.72
1:A:87:TYR:CE2	1:A:181:ILE:HG13	2.24	0.72
1:A:98:MET:HA	1:A:101:LEU:HD12	1.71	0.71
1:A:238:ARG:HE	1:A:238:ARG:CA	1.95	0.71
1:A:76:ASN:HB3	1:A:79:GLN:HG3	1.72	0.71
1:A:85:VAL:HG12	1:A:86:SER:N	2.06	0.70
1:A:372:GLN:HB2	4:A:719:HOH:O	1.91	0.70
1:A:121:HIS:HD2	4:A:791:HOH:O	1.74	0.70
1:A:63:ARG:HH11	1:A:63:ARG:CG	2.04	0.70
1:B:59:THR:O	1:B:63:ARG:HG2	1.92	0.70
1:B:61:LEU:HD11	1:B:239:THR:HG23	1.74	0.70
1:B:98:MET:HA	1:B:101:LEU:HD12	1.74	0.69
1:A:401:ALA:HA	4:A:672:HOH:O	1.92	0.69
1:B:166:ILE:HD11	4:B:634:HOH:O	1.90	0.69
1:B:419:HIS:CE1	1:B:442:ALA:HB2	2.27	0.69
1:A:181:ILE:O	1:A:182:ASP:C	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TYR:CD2	1:B:179:ASP:HB3	2.28	0.69
1:A:171:ARG:CZ	4:A:729:HOH:O	2.41	0.68
1:B:63:ARG:HH11	1:B:63:ARG:CG	2.05	0.68
1:B:162:ASP:O	1:B:166:ILE:HD12	1.94	0.68
1:B:183:CYS:SG	1:B:184:ASP:N	2.66	0.68
1:A:181:ILE:O	1:A:183:CYS:N	2.27	0.68
1:B:184:ASP:HB2	1:B:187:LYS:HG3	1.77	0.67
1:A:162:ASP:O	1:A:166:ILE:HD12	1.94	0.67
1:A:425:THR:HB	1:A:432:LYS:HG3	1.78	0.66
1:A:166:ILE:O	1:A:170:ILE:HG12	1.96	0.66
1:B:282:TYR:CE1	1:B:419:HIS:HA	2.30	0.66
1:A:184:ASP:OD1	1:A:187:LYS:HG3	1.95	0.66
1:A:419:HIS:CE1	1:A:442:ALA:HB2	2.30	0.65
1:B:166:ILE:O	1:B:170:ILE:HG12	1.97	0.65
1:B:111:ALA:O	1:B:115:VAL:HG23	1.96	0.65
1:B:185:ARG:CG	1:B:186:GLU:H	2.10	0.65
1:A:162:ASP:CB	1:A:165:ILE:HG13	2.28	0.64
1:A:282:TYR:CE1	1:A:419:HIS:HA	2.33	0.64
1:A:68:ILE:HG23	4:A:622:HOH:O	1.98	0.64
1:B:92:PHE:HE2	1:B:104:ARG:HD2	1.63	0.64
1:A:111:ALA:O	1:A:115:VAL:HG23	1.98	0.63
1:A:468:ALA:HB2	4:A:733:HOH:O	1.96	0.63
1:A:238:ARG:NE	1:A:238:ARG:CA	2.56	0.63
1:A:432:LYS:HE3	4:A:702:HOH:O	1.98	0.63
1:A:134:THR:HG22	1:A:203:TYR:CD1	2.33	0.63
1:B:425:THR:HB	1:B:432:LYS:HG3	1.79	0.63
1:B:185:ARG:CG	1:B:186:GLU:N	2.62	0.62
1:A:242:TYR:HD1	1:A:379:MET:HE1	1.65	0.61
1:B:134:THR:HG22	1:B:203:TYR:CD1	2.35	0.61
1:A:261:SER:O	1:A:264:ASN:HB2	2.01	0.61
1:A:117:ASN:HB2	4:A:791:HOH:O	2.01	0.61
1:B:87:TYR:CD2	1:B:88:LYS:N	2.69	0.61
1:A:106:GLN:OE1	1:A:106:GLN:HA	2.01	0.61
1:B:63:ARG:HE	1:B:405:ASP:HB2	1.66	0.60
1:B:354:GLN:HE22	1:B:455:ILE:HD13	1.67	0.60
1:B:234:HIS:O	1:B:238:ARG:HG2	2.01	0.60
1:B:452:ASN:ND2	1:B:457:ARG:HB2	2.16	0.60
1:A:68:ILE:HG12	4:A:622:HOH:O	2.01	0.60
1:A:125:HIS:C	4:A:656:HOH:O	2.39	0.60
1:A:184:ASP:CG	1:A:187:LYS:HB2	2.21	0.60
1:A:210:LEU:HD22	1:B:171:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:LYS:HA	4:B:671:HOH:O	2.03	0.59
1:B:187:LYS:HA	1:B:190:GLU:OE1	2.03	0.59
1:A:193:LEU:O	1:A:197:GLU:HG3	2.03	0.59
1:A:354:GLN:HE22	1:A:455:ILE:HD13	1.68	0.59
1:B:89:ASN:N	1:B:89:ASN:ND2	2.48	0.58
1:B:68:ILE:CD1	4:B:752:HOH:O	2.50	0.58
1:B:234:HIS:HD2	4:B:718:HOH:O	1.85	0.58
1:B:99:GLU:O	1:B:103:ILE:HD13	2.02	0.58
1:B:260:GLU:OE2	1:B:443:VAL:HG13	2.04	0.58
1:A:260:GLU:OE2	1:A:443:VAL:HG13	2.03	0.58
1:B:63:ARG:NH2	1:B:402:TYR:O	2.34	0.58
1:B:393:GLN:O	1:B:397:ARG:HG3	2.04	0.58
1:A:99:GLU:O	1:A:103:ILE:HD13	2.04	0.58
1:B:136:ARG:NH1	1:B:210:LEU:HB3	2.18	0.58
1:B:136:ARG:HG3	1:B:204:GLN:OE1	2.04	0.58
1:A:452:ASN:ND2	1:A:457:ARG:HB2	2.19	0.57
1:B:261:SER:O	1:B:264:ASN:HB2	2.04	0.57
1:A:251:ARG:HD3	1:A:385:GLU:O	2.04	0.57
1:A:136:ARG:NH1	1:A:210:LEU:HB3	2.19	0.57
1:B:353:ASP:HB3	1:B:453:VAL:HG12	1.87	0.57
1:B:162:ASP:CB	1:B:165:ILE:HG13	2.33	0.57
1:A:254:TYR:CE2	1:A:423:LYS:HG3	2.39	0.57
1:B:90:TYR:HB3	1:B:191:ASP:OD2	2.05	0.57
1:B:160:CYS:CB	4:B:634:HOH:O	2.46	0.57
1:B:106:GLN:OE1	1:B:106:GLN:HA	2.03	0.57
1:B:238:ARG:HE	1:B:238:ARG:CA	1.96	0.57
1:A:170:ILE:HG22	1:A:174:LYS:HB2	1.86	0.56
1:A:62:THR:HG23	1:A:72:THR:HG22	1.85	0.56
1:A:353:ASP:HB3	1:A:453:VAL:HG12	1.87	0.56
1:B:238:ARG:HG3	4:B:752:HOH:O	2.05	0.56
1:B:170:ILE:HG22	1:B:174:LYS:HB2	1.88	0.56
1:B:85:VAL:HG13	1:B:86:SER:O	2.06	0.56
1:B:92:PHE:CE2	1:B:104:ARG:HD2	2.40	0.56
1:A:263:LEU:HD22	1:A:268:ARG:HB2	1.87	0.56
1:A:287:ALA:O	1:A:291:GLN:HG3	2.07	0.55
1:B:173:VAL:HG21	3:B:503:AGS:H5'1	1.89	0.55
1:B:193:LEU:O	1:B:197:GLU:HG3	2.06	0.55
1:B:254:TYR:CE2	1:B:423:LYS:HG3	2.42	0.55
1:A:68:ILE:CG2	4:A:622:HOH:O	2.54	0.55
1:A:89:ASN:HB3	1:A:91:GLU:H	1.71	0.55
1:A:382:GLU:HG3	4:A:671:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLN:O	1:A:397:ARG:HG3	2.06	0.55
1:B:238:ARG:NE	1:B:238:ARG:CA	2.59	0.55
1:A:180:TYR:O	1:A:182:ASP:N	2.40	0.55
1:A:383:ARG:NH2	4:A:753:HOH:O	2.39	0.54
1:B:189:LEU:HD12	1:B:193:LEU:HG	1.88	0.54
1:A:134:THR:HG22	1:A:203:TYR:CE1	2.42	0.54
1:A:234:HIS:O	1:A:238:ARG:HG2	2.08	0.54
1:B:89:ASN:N	1:B:89:ASN:HD22	2.05	0.54
1:A:39:ASN:HB3	4:A:780:HOH:O	2.07	0.54
1:A:258:HIS:CD2	1:A:258:HIS:H	2.25	0.54
1:B:258:HIS:H	1:B:258:HIS:CD2	2.25	0.53
1:B:344:HIS:HE1	4:B:792:HOH:O	1.91	0.53
1:B:411:LEU:HD12	1:B:411:LEU:C	2.29	0.53
1:A:180:TYR:O	1:A:181:ILE:C	2.46	0.53
1:B:185:ARG:HG3	1:B:186:GLU:H	1.73	0.53
1:B:287:ALA:O	1:B:291:GLN:HG3	2.09	0.53
1:A:173:VAL:HG21	3:A:503:AGS:H5'1	1.89	0.53
1:B:88:LYS:H	1:B:89:ASN:ND2	2.07	0.53
1:B:110:ALA:O	1:B:113:LYS:HB2	2.09	0.53
1:A:79:GLN:NE2	4:A:758:HOH:O	2.38	0.53
1:A:98:MET:HB3	4:A:763:HOH:O	2.08	0.53
1:A:468:ALA:CB	4:A:733:HOH:O	2.55	0.53
1:B:419:HIS:ND1	1:B:442:ALA:HB2	2.24	0.53
1:A:136:ARG:HG3	1:A:204:GLN:OE1	2.10	0.52
1:A:230:ARG:HH11	1:A:230:ARG:CG	2.22	0.52
1:B:263:LEU:HD22	1:B:268:ARG:HB2	1.91	0.52
1:A:173:VAL:HG11	1:A:429:TYR:CZ	2.44	0.52
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.22	0.52
1:A:357:TYR:HD2	1:A:358:ARG:HH11	1.58	0.52
1:B:62:THR:HG23	1:B:72:THR:HG22	1.90	0.52
1:A:106:GLN:OE1	1:A:106:GLN:CA	2.56	0.52
1:A:180:TYR:CD2	1:A:188:VAL:HG13	2.44	0.52
1:A:61:LEU:HD11	1:A:239:THR:CG2	2.37	0.52
1:B:61:LEU:HD11	1:B:239:THR:CG2	2.40	0.52
1:B:251:ARG:HD3	1:B:385:GLU:O	2.10	0.52
1:B:357:TYR:HD2	1:B:358:ARG:HH11	1.58	0.52
1:A:411:LEU:C	1:A:411:LEU:HD12	2.30	0.52
1:A:110:ALA:O	1:A:113:LYS:HB2	2.09	0.51
1:B:184:ASP:O	1:B:185:ARG:O	2.28	0.51
1:B:437:TYR:CE2	1:B:439:ASN:HA	2.46	0.51
1:A:210:LEU:HB3	1:B:171:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ALA:HA	4:B:647:HOH:O	2.09	0.51
1:B:106:GLN:OE1	1:B:106:GLN:CA	2.58	0.51
1:B:231:VAL:HG13	1:B:236:GLN:HB3	1.92	0.51
1:A:437:TYR:CE2	1:A:439:ASN:HA	2.46	0.51
1:A:266:ARG:NH2	4:A:697:HOH:O	2.43	0.51
1:B:121:HIS:CE1	4:B:791:HOH:O	2.63	0.51
1:B:134:THR:HG22	1:B:203:TYR:CE1	2.45	0.51
1:A:147:LYS:HG2	4:A:708:HOH:O	2.11	0.51
1:A:189:LEU:HD12	1:A:193:LEU:HG	1.92	0.51
1:B:90:TYR:N	1:B:191:ASP:OD2	2.44	0.51
1:A:227:MET:HE1	4:A:743:HOH:O	2.10	0.50
1:A:376:PRO:HD3	4:A:659:HOH:O	2.11	0.50
1:A:184:ASP:CG	1:A:187:LYS:HG3	2.32	0.50
1:A:197:GLU:HA	1:A:200:GLU:HG3	1.91	0.50
1:A:419:HIS:ND1	1:A:442:ALA:HB2	2.27	0.50
1:B:55:THR:OG1	3:B:503:AGS:PG	2.70	0.50
1:B:358:ARG:HD2	4:B:771:HOH:O	2.11	0.50
1:A:455:ILE:CD1	4:A:695:HOH:O	2.59	0.49
1:B:330:ALA:HA	4:B:766:HOH:O	2.11	0.49
1:A:231:VAL:HG13	1:A:236:GLN:HB3	1.94	0.49
1:B:141:LEU:O	1:B:144:GLN:HB3	2.13	0.49
1:B:88:LYS:HE2	1:B:180:TYR:HD2	1.76	0.49
1:A:49:LEU:HB2	1:A:52:ARG:HD3	1.94	0.49
1:A:163:PRO:HD3	4:A:701:HOH:O	2.12	0.49
1:A:216:TYR:CD1	1:A:216:TYR:C	2.86	0.49
1:B:216:TYR:CD1	1:B:216:TYR:C	2.86	0.49
1:A:404:LEU:HB2	4:A:672:HOH:O	2.12	0.49
1:A:117:ASN:CB	4:A:791:HOH:O	2.60	0.48
1:A:457:ARG:NE	1:A:462:ALA:HB2	2.29	0.48
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.66	0.48
1:B:90:TYR:CD2	1:B:194:LYS:HD3	2.49	0.48
1:A:382:GLU:CG	4:A:671:HOH:O	2.59	0.48
1:A:54:LYS:HE3	1:A:132:THR:HA	1.96	0.47
1:B:48:GLY:HA2	4:B:627:HOH:O	2.12	0.47
1:B:82:ARG:HD3	1:B:179:ASP:OD1	2.14	0.47
1:B:41:PRO:HB2	1:B:119:LEU:HD13	1.96	0.47
1:B:63:ARG:HH11	1:B:63:ARG:HG3	1.77	0.47
1:B:408:SER:O	1:B:412:PRO:HD3	2.14	0.47
1:B:242:TYR:HD1	1:B:379:MET:HE1	1.78	0.47
1:A:161:ASN:C	4:A:701:HOH:O	2.53	0.47
1:A:184:ASP:CB	1:A:187:LYS:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:THR:OG1	3:B:503:AGS:O3G	2.32	0.47
1:B:327:GLU:OE1	1:B:394:ALA:HB3	2.15	0.47
1:A:448:GLU:HG3	4:A:635:HOH:O	2.13	0.47
1:A:296:SER:O	1:A:297:SER:C	2.53	0.47
1:A:408:SER:O	1:A:412:PRO:HD3	2.15	0.47
1:A:122:GLU:O	1:A:123:GLU:HB2	2.15	0.46
1:B:173:VAL:HG11	1:B:429:TYR:CZ	2.50	0.46
1:B:457:ARG:NE	1:B:462:ALA:HB2	2.30	0.46
1:A:68:ILE:HG22	1:A:375:GLU:CG	2.45	0.46
1:A:85:VAL:CG1	1:A:86:SER:H	2.18	0.46
1:A:425:THR:HB	1:A:432:LYS:CG	2.45	0.46
1:A:163:PRO:CD	4:A:701:HOH:O	2.63	0.46
1:B:184:ASP:HB3	1:B:185:ARG:H	1.36	0.46
1:B:61:LEU:HD22	1:B:65:LEU:HG	1.96	0.46
1:B:49:LEU:HB2	1:B:52:ARG:HD3	1.95	0.46
1:B:197:GLU:HA	1:B:200:GLU:HG3	1.98	0.46
1:A:90:TYR:CD1	1:A:90:TYR:C	2.88	0.46
1:A:287:ALA:HB2	1:A:315:LEU:HD23	1.98	0.46
1:A:378:ILE:HD12	1:A:402:TYR:CG	2.51	0.46
1:B:103:ILE:N	1:B:103:ILE:CD1	2.79	0.46
1:A:141:LEU:O	1:A:144:GLN:HB3	2.16	0.46
1:B:415:LYS:CE	4:B:699:HOH:O	2.55	0.45
1:B:144:GLN:CD	4:B:702:HOH:O	2.54	0.45
1:B:238:ARG:HD2	4:B:633:HOH:O	2.15	0.45
1:A:213:HIS:HB3	1:B:186:GLU:OE2	2.17	0.45
1:B:116:HIS:O	1:B:120:SER:HB2	2.17	0.45
1:A:327:GLU:OE1	1:A:394:ALA:HB3	2.16	0.45
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.82	0.45
1:B:361:TYR:HE1	4:B:639:HOH:O	1.99	0.45
1:A:98:MET:CB	4:A:763:HOH:O	2.64	0.45
1:B:92:PHE:C	1:B:92:PHE:CD2	2.89	0.45
1:A:55:THR:OG1	3:A:503:AGS:O3G	2.35	0.45
1:B:207:ASP:O	1:B:211:ASP:HB2	2.16	0.45
1:A:41:PRO:HB2	1:A:119:LEU:HD13	1.98	0.45
1:A:451:GLU:HG3	4:A:657:HOH:O	2.17	0.45
1:B:379:MET:HB2	1:B:379:MET:HE3	1.87	0.45
1:B:88:LYS:HA	1:B:88:LYS:HD3	1.76	0.45
1:A:184:ASP:HB3	1:A:187:LYS:HB2	1.99	0.44
1:A:230:ARG:HH11	1:A:230:ARG:HG3	1.82	0.44
1:A:140:SER:HB3	1:B:163:PRO:HD2	2.00	0.44
1:B:79:GLN:NE2	4:B:796:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:CD2	1:B:92:PHE:O	2.71	0.44
1:B:193:LEU:HA	1:B:193:LEU:HD23	1.66	0.44
1:B:425:THR:HB	1:B:432:LYS:CG	2.47	0.44
1:A:56:TYR:CD2	3:A:503:AGS:H8	2.53	0.44
1:B:63:ARG:CB	1:B:63:ARG:CZ	2.96	0.44
1:B:54:LYS:HE3	1:B:132:THR:HA	2.00	0.44
1:B:327:GLU:HB2	1:B:392:HIS:CG	2.53	0.44
1:A:147:LYS:HE2	4:A:708:HOH:O	2.18	0.44
1:B:87:TYR:CD1	1:B:89:ASN:ND2	2.86	0.44
1:A:96:ASP:C	1:A:96:ASP:OD1	2.56	0.43
1:B:221:ASP:OD1	4:B:667:HOH:O	2.21	0.43
1:A:61:LEU:HD22	1:A:65:LEU:HG	1.99	0.43
1:B:287:ALA:HB2	1:B:315:LEU:HD23	2.00	0.43
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.90	0.43
1:A:309:ILE:O	1:A:313:GLU:HG2	2.18	0.43
1:B:96:ASP:OD1	1:B:96:ASP:C	2.55	0.43
1:B:103:ILE:CD1	1:B:103:ILE:H	2.32	0.43
1:A:185:ARG:HB3	1:A:186:GLU:H	1.26	0.43
1:B:90:TYR:CE2	1:B:91:GLU:HG2	2.53	0.43
1:B:232:GLN:HG3	1:B:236:GLN:OE1	2.17	0.43
1:B:287:ALA:CB	1:B:315:LEU:HD23	2.49	0.43
1:A:287:ALA:CB	1:A:315:LEU:HD23	2.49	0.43
1:A:458:GLU:HB3	1:A:459:PRO:HD2	2.01	0.43
1:B:39:ASN:N	4:B:733:HOH:O	2.51	0.43
1:B:90:TYR:CD1	1:B:90:TYR:C	2.92	0.43
1:A:64:TYR:CD2	4:A:622:HOH:O	2.69	0.43
1:B:234:HIS:CD2	4:B:718:HOH:O	2.67	0.43
1:B:296:SER:O	1:B:297:SER:C	2.56	0.43
1:A:63:ARG:CB	1:A:63:ARG:CZ	2.97	0.43
1:A:116:HIS:O	1:A:120:SER:HB2	2.18	0.43
1:B:422:LEU:HD22	1:B:435:SER:HA	2.00	0.43
1:A:232:GLN:HG3	1:A:236:GLN:OE1	2.18	0.43
1:B:290:ILE:HD13	1:B:290:ILE:HA	1.89	0.43
1:B:411:LEU:C	1:B:411:LEU:CD1	2.87	0.43
1:B:309:ILE:O	1:B:313:GLU:HG2	2.19	0.42
1:A:86:SER:OG	1:A:87:TYR:HD1	2.02	0.42
1:B:180:TYR:C	1:B:181:ILE:O	2.57	0.42
1:B:117:ASN:ND2	1:B:122:GLU:OE2	2.45	0.42
1:B:185:ARG:HG2	1:B:186:GLU:N	2.33	0.42
1:A:103:ILE:N	1:A:103:ILE:CD1	2.82	0.42
1:A:409:GLU:HA	4:A:623:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:O	1:B:187:LYS:C	2.58	0.42
1:B:239:THR:O	1:B:243:LEU:HG	2.19	0.42
1:B:458:GLU:HB3	1:B:459:PRO:HD2	2.01	0.42
1:A:117:ASN:ND2	1:A:122:GLU:OE2	2.44	0.42
1:A:352:ARG:CZ	4:A:637:HOH:O	2.68	0.42
1:B:264:ASN:HD22	1:B:264:ASN:HA	1.67	0.42
1:B:87:TYR:CD2	1:B:87:TYR:C	2.93	0.42
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.82	0.42
1:A:163:PRO:N	4:A:701:HOH:O	2.53	0.42
1:B:71:PRO:HD2	1:B:125:HIS:CG	2.55	0.42
1:A:411:LEU:C	1:A:411:LEU:CD1	2.89	0.41
1:B:325:LEU:O	1:B:395:VAL:HG21	2.20	0.41
1:A:87:TYR:CE2	1:A:181:ILE:CG1	2.98	0.41
1:A:379:MET:HB2	1:A:379:MET:HE3	1.87	0.41
1:B:263:LEU:HG	1:B:273:SER:HB3	2.02	0.41
1:B:337:THR:HG23	1:B:340:GLU:OE1	2.20	0.41
1:A:268:ARG:HG2	1:A:337:THR:HG22	2.02	0.41
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.91	0.41
1:A:71:PRO:HD2	1:A:125:HIS:CG	2.55	0.41
1:A:444:ASN:ND2	1:A:467:PRO:HB3	2.36	0.41
1:B:444:ASN:ND2	1:B:467:PRO:HB3	2.35	0.41
1:A:366:SER:H	1:A:369:ASP:HB2	1.85	0.41
1:B:77:LEU:HD23	1:B:77:LEU:HA	1.86	0.41
1:B:81:ARG:O	1:B:84:ALA:HB3	2.20	0.41
1:B:101:LEU:O	1:B:105:LYS:HB2	2.20	0.41
1:A:268:ARG:NH1	1:A:340:GLU:OE1	2.53	0.41
1:A:55:THR:OG1	3:A:503:AGS:PG	2.79	0.41
1:A:121:HIS:CD2	4:A:791:HOH:O	2.57	0.41
1:A:207:ASP:O	1:A:211:ASP:HB2	2.21	0.41
1:A:325:LEU:O	1:A:395:VAL:HG21	2.20	0.41
1:B:85:VAL:HG13	1:B:86:SER:H	1.82	0.41
1:B:238:ARG:CZ	4:B:713:HOH:O	2.69	0.41
1:B:258:HIS:HD2	1:B:391:CYS:O	2.04	0.41
1:B:63:ARG:NE	1:B:405:ASP:HB2	2.33	0.41
1:B:282:TYR:CD1	1:B:419:HIS:HA	2.56	0.41
1:B:358:ARG:HH11	1:B:358:ARG:HG3	1.86	0.41
1:B:379:MET:HA	1:B:379:MET:CE	2.51	0.41
1:A:337:THR:HG23	1:A:340:GLU:OE1	2.21	0.40
1:B:76:ASN:HB3	4:B:796:HOH:O	2.21	0.40
1:A:62:THR:OG1	1:A:74:VAL:HG23	2.22	0.40
1:A:264:ASN:HA	4:A:652:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PHE:CZ	1:A:436:ILE:HD13	2.57	0.40
1:B:268:ARG:HG2	1:B:337:THR:HG22	2.03	0.40
1:A:98:MET:CG	4:A:763:HOH:O	2.70	0.40
1:A:103:ILE:CD1	1:A:103:ILE:H	2.35	0.40
1:B:103:ILE:N	1:B:103:ILE:HD12	2.37	0.40
1:A:327:GLU:HB2	1:A:392:HIS:CG	2.56	0.40
1:B:183:CYS:SG	1:B:188:VAL:CG2	3.09	0.40
1:B:352:ARG:NH2	2:B:502:PO4:O1	2.54	0.40
1:B:378:ILE:HD12	1:B:402:TYR:CG	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:730:HOH:O	4:B:691:HOH:O[4_456]	1.88	0.32

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/432 (100%)	396 (92%)	26 (6%)	8 (2%)	8	10
1	B	430/432 (100%)	395 (92%)	28 (6%)	7 (2%)	9	13
All	All	860/864 (100%)	791 (92%)	54 (6%)	15 (2%)	9	11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	B	88	LYS
1	B	185	ARG
1	A	88	LYS

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Mol	Chain	Res	Type
1	A	182	ASP
1	A	297	SER
1	A	429	TYR
1	B	89	ASN
1	B	181	ILE
1	B	297	SER
1	B	429	TYR
1	A	181	ILE
1	A	86	SER
1	B	91	GLU
1	A	71	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/388 (100%)	346 (89%)	42 (11%)	6	9
1	B	388/388 (100%)	341 (88%)	47 (12%)	5	6
All	All	776/776 (100%)	687 (88%)	89 (12%)	5	7

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	58	SER
1	A	61	LEU
1	A	63	ARG
1	A	98	MET
1	A	103	ILE
1	A	105	LYS
1	A	106	GLN
1	A	117	ASN
1	A	134	THR
1	A	141	LEU
1	A	144	GLN

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Mol	Chain	Res	Type
1	A	165	ILE
1	A	170	ILE
1	A	171	ARG
1	A	173	VAL
1	A	184	ASP
1	A	185	ARG
1	A	186	GLU
1	A	189	LEU
1	A	190	GLU
1	A	209	GLU
1	A	212	SER
1	A	222	VAL
1	A	230	ARG
1	A	235	ILE
1	A	237	SER
1	A	238	ARG
1	A	251	ARG
1	A	264	ASN
1	A	265	ILE
1	A	277	VAL
1	A	292	SER
1	A	323	LYS
1	A	379	MET
1	A	411	LEU
1	A	422	LEU
1	A	429	TYR
1	A	432	LYS
1	A	451	GLU
1	A	455	ILE
1	A	460	GLU
1	B	58	SER
1	B	61	LEU
1	B	63	ARG
1	B	85	VAL
1	B	88	LYS
1	B	89	ASN
1	B	90	TYR
1	B	98	MET
1	B	102	GLN
1	B	103	ILE
1	B	105	LYS
1	B	106	GLN

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Mol	Chain	Res	Type
1	B	117	ASN
1	B	134	THR
1	B	141	LEU
1	B	144	GLN
1	B	165	ILE
1	B	170	ILE
1	B	171	ARG
1	B	173	VAL
1	B	181	ILE
1	B	183	CYS
1	B	185	ARG
1	B	186	GLU
1	B	189	LEU
1	B	190	GLU
1	B	209	GLU
1	B	212	SER
1	B	222	VAL
1	B	230	ARG
1	B	235	ILE
1	B	237	SER
1	B	238	ARG
1	B	251	ARG
1	B	264	ASN
1	B	265	ILE
1	B	277	VAL
1	B	292	SER
1	B	323	LYS
1	B	379	MET
1	B	411	LEU
1	B	422	LEU
1	B	429	TYR
1	B	432	LYS
1	B	451	GLU
1	B	455	ILE
1	B	460	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	116	HIS
1	A	169	ASN

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Mol	Chain	Res	Type
1	A	354	GLN
1	B	89	ASN
1	B	116	HIS
1	B	144	GLN
1	B	169	ASN
1	B	354	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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	PO4	B	501	-	4,4,4	1.24	0	6,6,6	0.40	0
2	PO4	A	501	-	4,4,4	1.34	1 (25%)	6,6,6	0.83	0
2	PO4	A	502	-	4,4,4	2.20	2 (50%)	6,6,6	0.71	0
2	PO4	B	502	-	4,4,4	1.80	1 (25%)	6,6,6	0.67	0
3	AGS	B	503	-	26,33,33	1.97	9 (34%)	26,52,52	1.89	6 (23%)
3	AGS	A	503	-	26,33,33	2.10	8 (30%)	26,52,52	1.52	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	B	503	-	-	3/17/38/38	0/3/3/3
3	AGS	A	503	-	-	5/17/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	AGS	PG-S1G	-6.15	1.77	1.90
3	A	503	AGS	C6-N6	4.08	1.49	1.34
3	B	503	AGS	C6-N6	3.98	1.48	1.34
3	B	503	AGS	C2-N3	3.89	1.38	1.32
3	A	503	AGS	O4'-C1'	-3.66	1.36	1.41
3	B	503	AGS	O4'-C1'	-3.53	1.36	1.41
3	A	503	AGS	O4'-C4'	-3.45	1.37	1.45
3	B	503	AGS	PG-S1G	-3.17	1.83	1.90
2	A	502	PO4	P-O3	-3.06	1.45	1.54
3	B	503	AGS	O5'-C5'	-2.90	1.33	1.44
2	B	502	PO4	P-O1	2.89	1.57	1.50
3	A	503	AGS	C2'-C1'	-2.71	1.49	1.53
3	B	503	AGS	C4-N3	2.61	1.39	1.35
3	B	503	AGS	PA-O5'	-2.42	1.49	1.59
3	A	503	AGS	C2-N3	2.36	1.35	1.32
2	A	502	PO4	P-O4	2.32	1.61	1.54
2	A	501	PO4	P-O4	-2.25	1.47	1.54
3	B	503	AGS	O3'-C3'	2.24	1.48	1.43
3	A	503	AGS	O5'-C5'	-2.10	1.36	1.44
3	B	503	AGS	O4'-C4'	-2.08	1.40	1.45
3	A	503	AGS	PB-O2B	-2.04	1.45	1.55

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	AGS	O4'-C1'-C2'	-6.79	97.01	106.93
3	A	503	AGS	PA-O3A-PB	-4.02	119.04	132.83
3	B	503	AGS	O4'-C4'-C3'	-3.22	98.74	105.11
3	B	503	AGS	PA-O3A-PB	-2.64	123.77	132.83
3	B	503	AGS	O3'-C3'-C4'	-2.48	103.89	111.05
3	A	503	AGS	O3'-C3'-C2'	-2.37	104.16	111.82
3	A	503	AGS	O2'-C2'-C1'	-2.27	102.49	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	AGS	O4'-C1'-C2'	-2.16	103.77	106.93
3	A	503	AGS	C5-C6-N6	2.11	123.56	120.35
3	B	503	AGS	O2A-PA-O1A	2.09	122.57	112.24
3	B	503	AGS	O2'-C2'-C1'	-2.01	103.42	110.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	AGS	PB-O3B-PG-O2G
3	A	503	AGS	PB-O3B-PG-O3G
3	B	503	AGS	PB-O3B-PG-O2G
3	B	503	AGS	PB-O3B-PG-O3G
3	B	503	AGS	C5'-O5'-PA-O2A
3	A	503	AGS	C5'-O5'-PA-O3A
3	A	503	AGS	PA-O3A-PB-O2B
3	A	503	AGS	C5'-O5'-PA-O2A

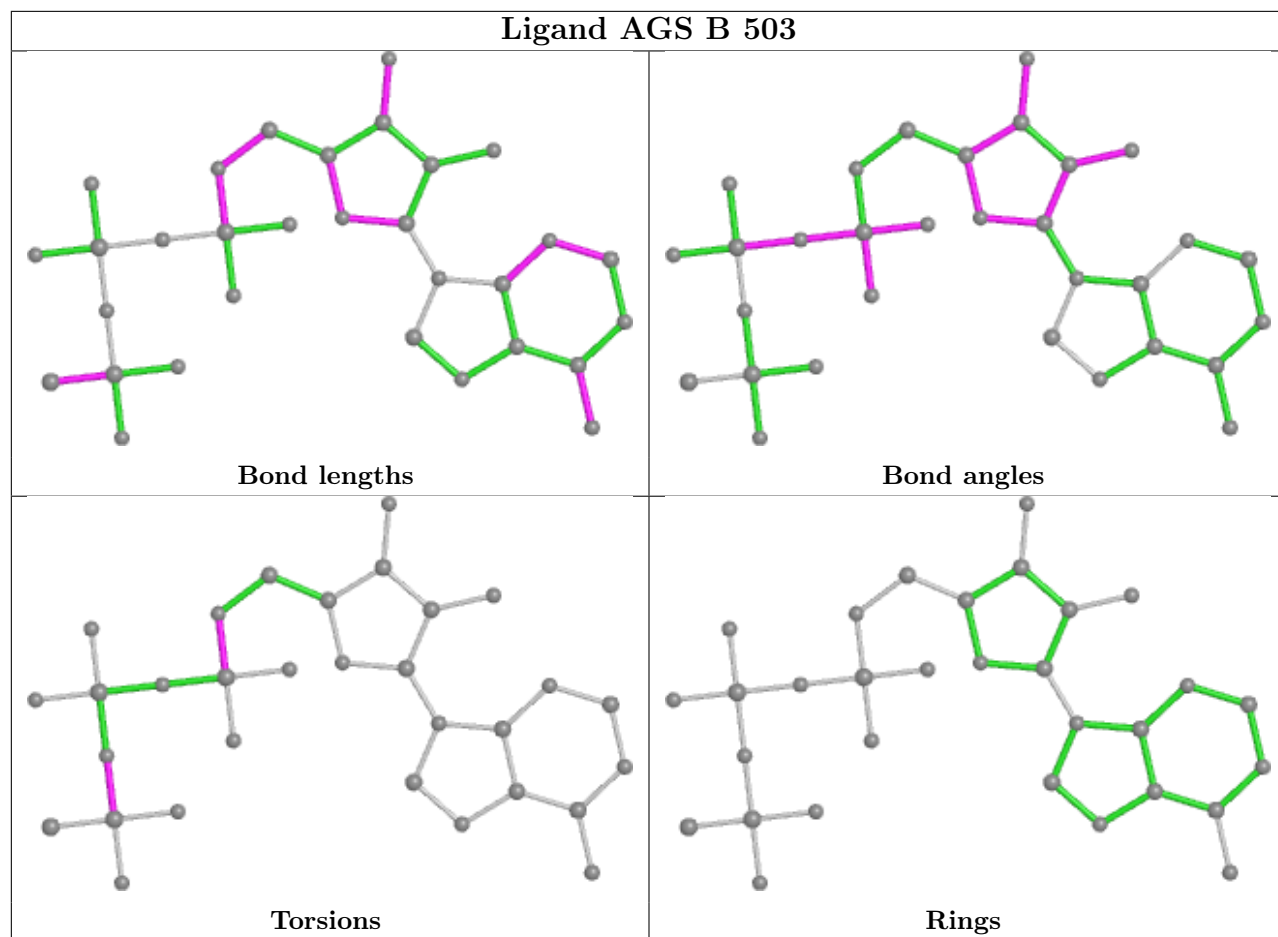
There are no ring outliers.

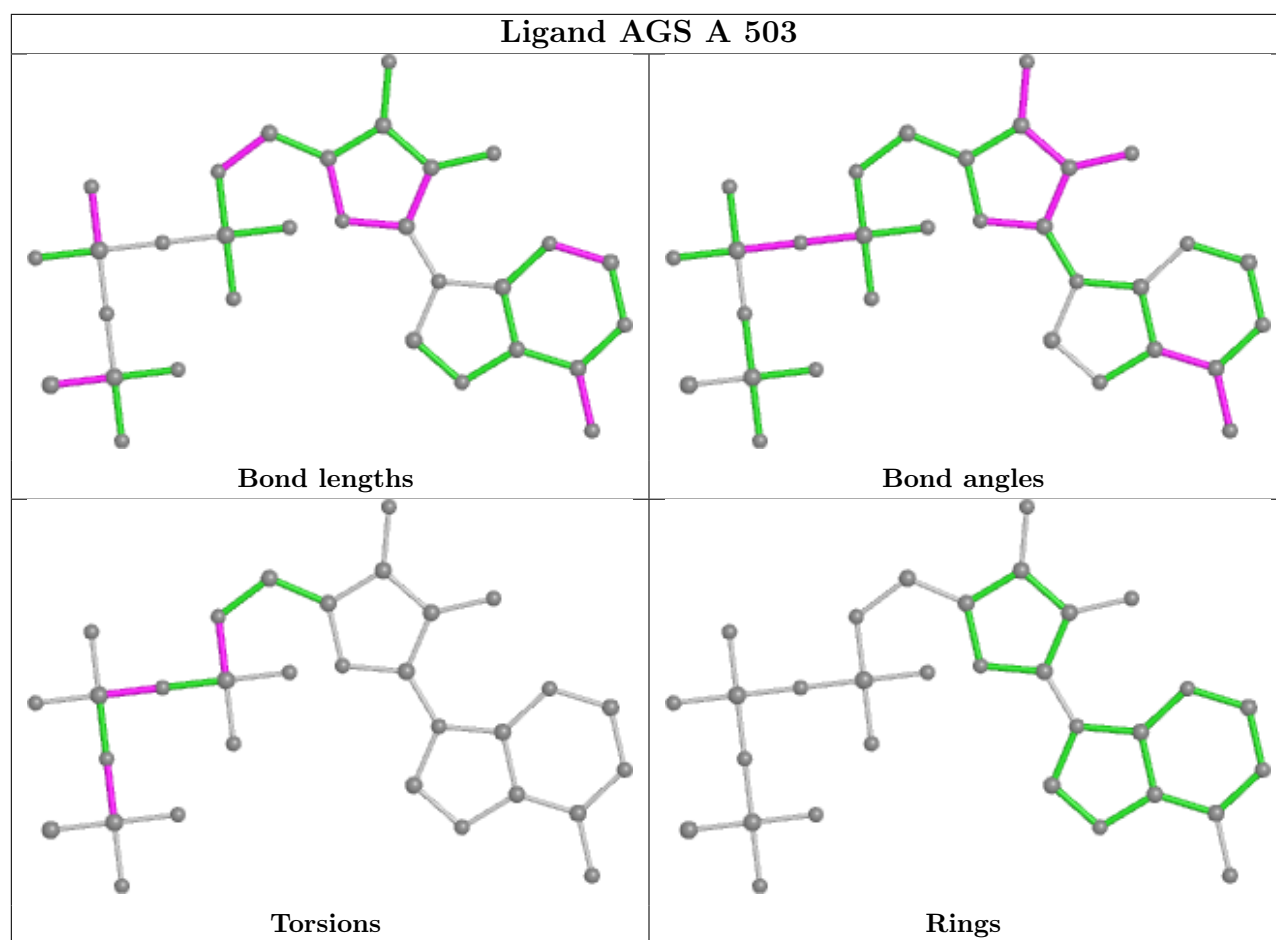
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	PO4	1	0
3	B	503	AGS	3	0
3	A	503	AGS	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 than 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 AGS B 503





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	432/432 (100%)	-0.17	15 (3%) 44 43	22, 38, 76, 95	0
1	B	432/432 (100%)	-0.20	13 (3%) 50 49	21, 37, 75, 95	0
All	All	864/864 (100%)	-0.19	28 (3%) 47 46	21, 37, 76, 95	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	ILE	6.0
1	B	98	MET	5.8
1	B	181	ILE	5.0
1	B	470	TYR	3.7
1	A	88	LYS	3.5
1	A	92	PHE	3.5
1	A	470	TYR	3.4
1	A	182	ASP	3.3
1	A	178	PRO	3.2
1	B	185	ARG	3.1
1	A	87	TYR	2.7
1	B	94	LEU	2.7
1	A	185	ARG	2.7
1	A	183	CYS	2.7
1	A	94	LEU	2.7
1	A	455	ILE	2.7
1	A	187	LYS	2.5
1	B	106	GLN	2.5
1	A	194	LYS	2.4
1	B	186	GLU	2.3
1	B	88	LYS	2.3
1	A	103	ILE	2.3
1	B	187	LYS	2.2
1	B	184	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	175	LEU	2.1
1	B	177	SER	2.1
1	B	132	THR	2.1
1	A	132	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

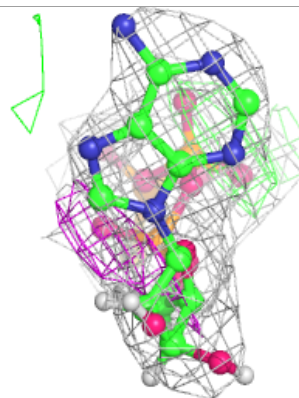
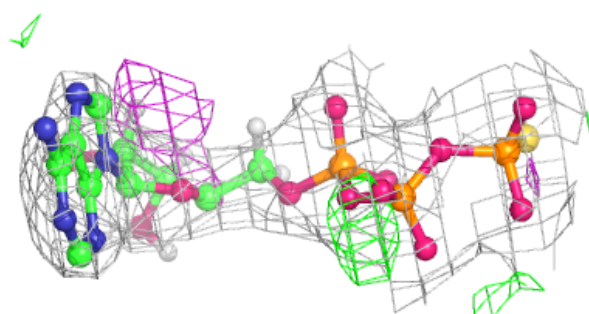
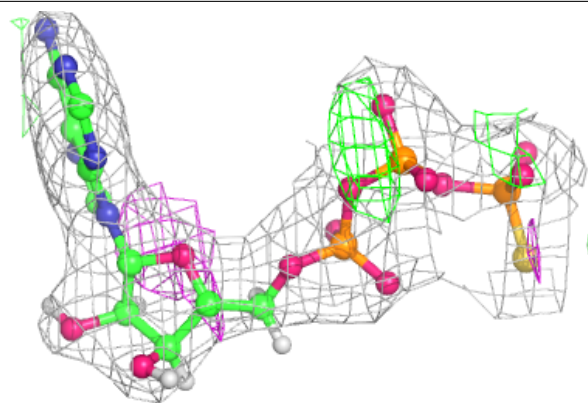
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AGS	A	503	31/31	0.90	0.18	20,55,61,64	0
3	AGS	B	503	31/31	0.94	0.14	20,40,57,60	0
2	PO4	A	502	5/5	0.98	0.17	22,22,26,26	0
2	PO4	B	501	5/5	0.98	0.23	28,29,30,33	0
2	PO4	A	501	5/5	0.99	0.17	30,32,32,32	0
2	PO4	B	502	5/5	0.99	0.20	23,26,29,32	0

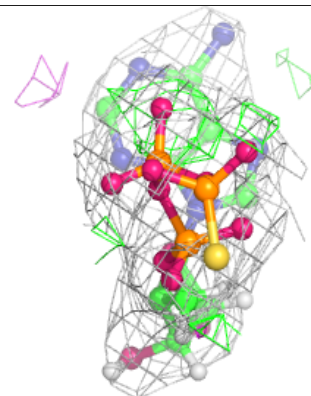
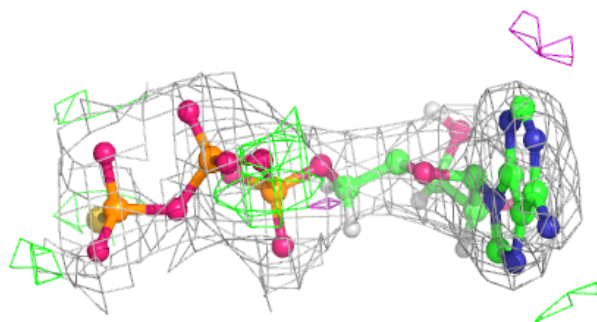
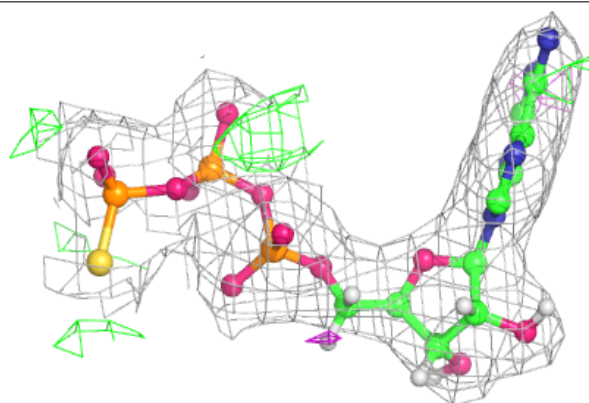
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AGS A 503:**

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

**Electron density around AGS B 503:**

$2mF_o-DF_c$  (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.