Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 03:56 PM EST

PDB ID	:	3THX
Title	:	Human MutSbeta complexed with an IDL of 3 bases (Loop3) and ADP
Authors	:	Yang, W.
Deposited on	:	2011-08-19
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

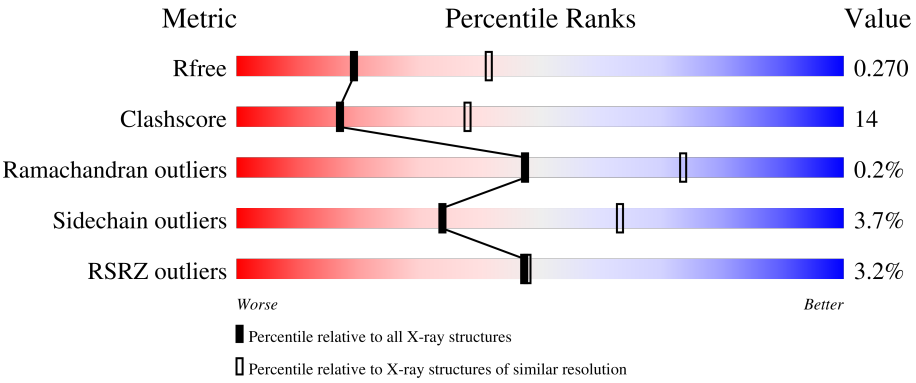
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	934	4% 63% 29% · 7%
2	B	918	2% 63% 28% · 7%
3	D	24	8% 25% 63% 12%
4	E	25	12% 44% 56%

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
6	NA	B	1	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14645 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	868	6795	4320	1153	1286	36	0	5	0

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	852	6796	4336	1158	1269	33	1	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	208	GLY	-	expression tag	GB 119616268
B	209	PRO	-	expression tag	GB 119616268

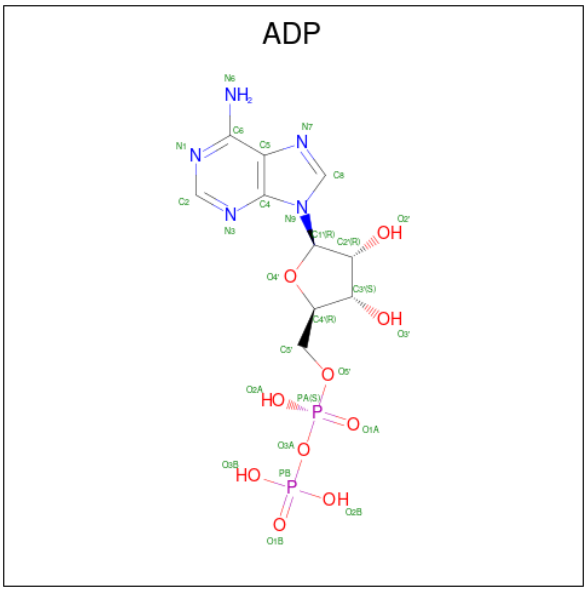
- Molecule 3 is a DNA chain called DNA Loop3 minus strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	21	427	205	77	125	20	0	0	0

- Molecule 4 is a DNA chain called DNA Loop3 plus strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	E	25	572	273	108	164	27	0	3	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

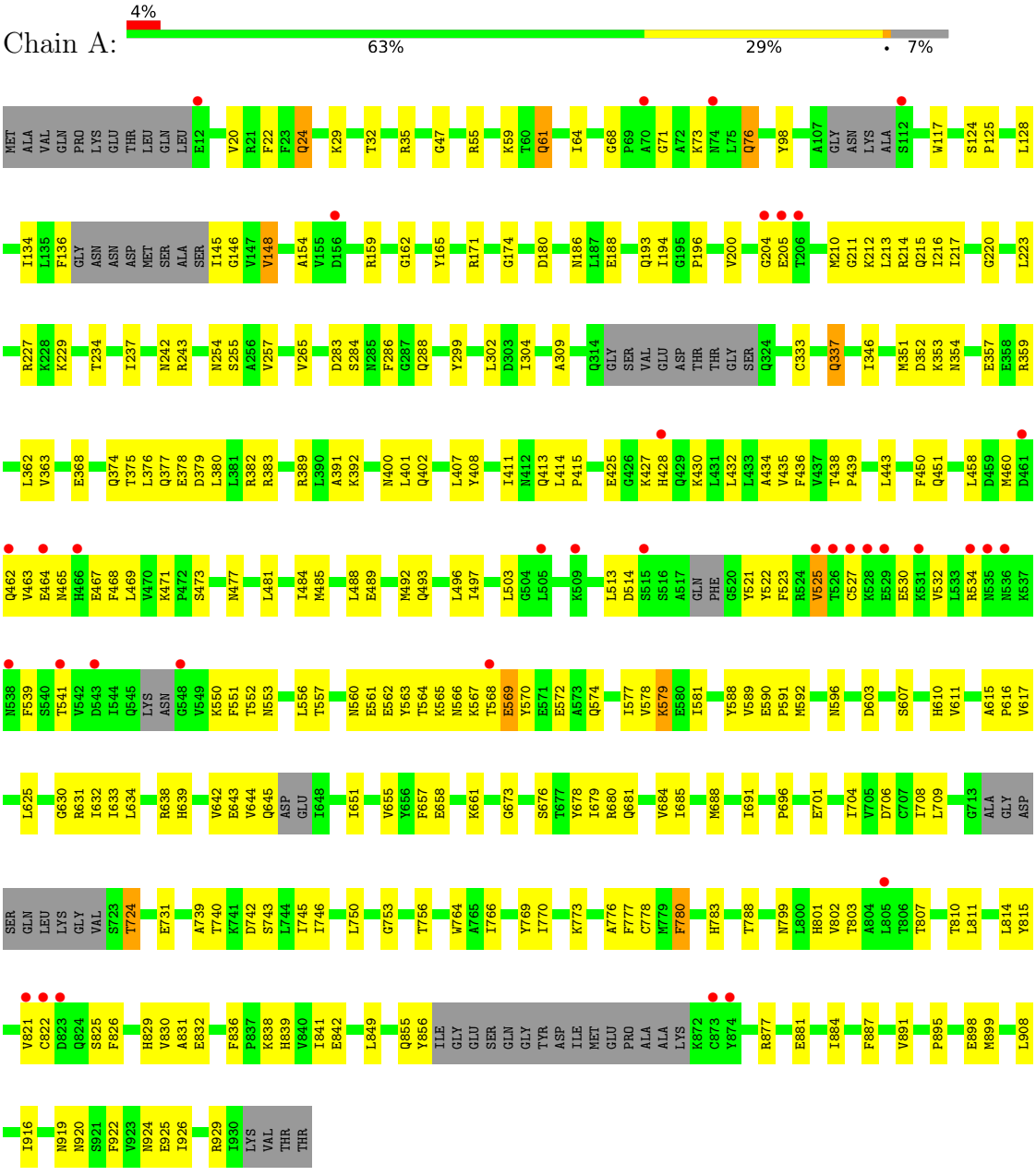
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	O	0	0
			8	8		
7	B	19	Total	O	0	0
			19	19		

3 Residue-property plots (i)

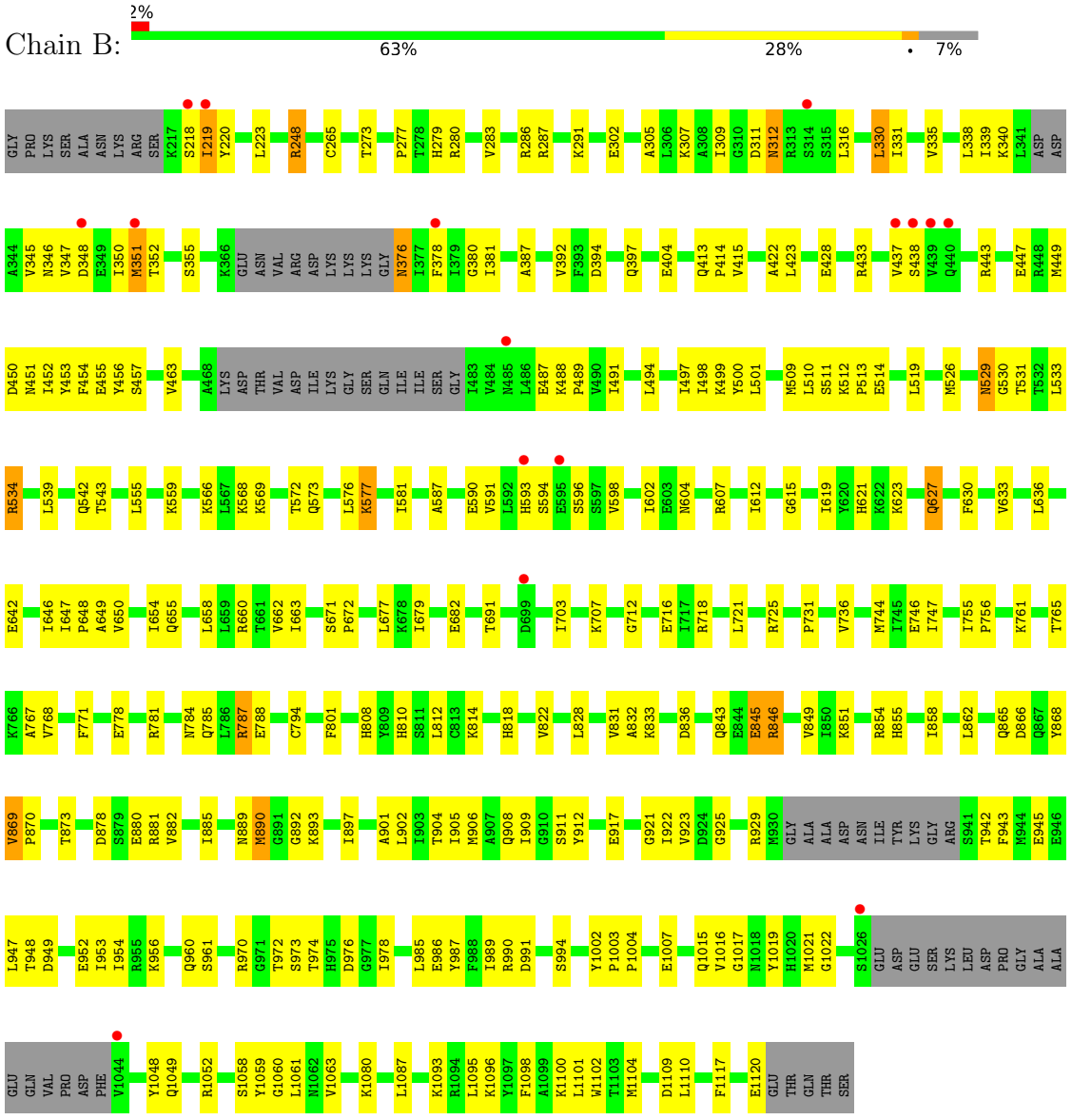
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA mismatch repair protein Msh2

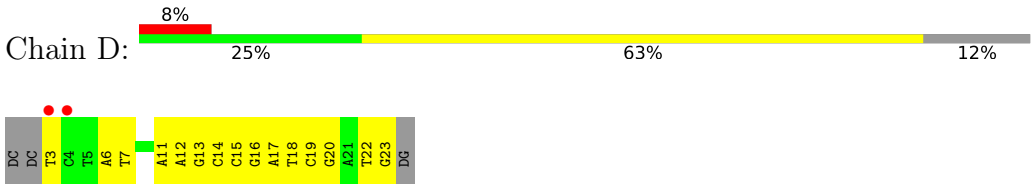
Chain A:



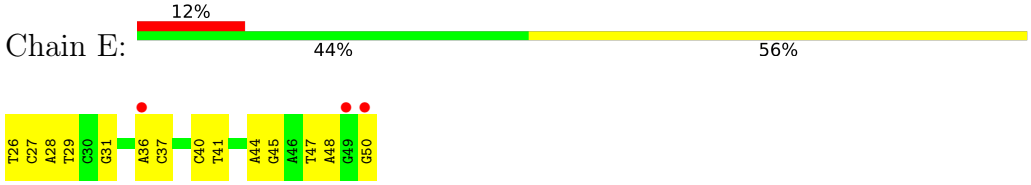
• Molecule 2: DNA mismatch repair protein Msh3



• Molecule 3: DNA Loop3 minus strand



• Molecule 4: DNA Loop3 plus strand



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.12Å 91.54Å 95.58Å 67.88° 86.51° 72.86°	Depositor
Resolution (Å)	27.00 – 2.70 29.12 – 2.69	Depositor EDS
% Data completeness (in resolution range)	89.9 (27.00-2.70) 86.1 (29.12-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.63 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486), CNS	Depositor
R, R_{free}	0.210 , 0.273 0.207 , 0.270	Depositor DCC
R_{free} test set	1522 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å^2)	51.2	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14645	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.23	0/6913	0.37	0/9322
2	B	0.23	0/6943	0.38	0/9383
3	D	0.43	0/478	1.00	0/736
4	E	0.45	0/642	1.00	0/989
All	All	0.25	0/14976	0.46	0/20430

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6795	0	6784	192	0
2	B	6796	0	6848	200	0
3	D	427	0	239	15	0
4	E	572	0	316	13	0
5	A	27	0	12	0	0
6	B	1	0	0	0	0
7	A	8	0	0	0	0
7	B	19	0	0	0	0
All	All	14645	0	14199	402	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 14.

All (402) 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)
2:B:787:ARG:HG2	2:B:787:ARG:HH11	1.13	1.12
3:D:3:DT:H3	4:E:50:DG:H1	1.09	0.94
2:B:865:GLN:HE21	2:B:868:TYR:H	1.17	0.92
1:A:204:GLY:HA3	1:A:229:LYS:HE3	1.52	0.91
1:A:76:GLN:H	1:A:76:GLN:HE21	1.19	0.89
1:A:503:LEU:HD21	1:A:539:PHE:HE2	1.42	0.83
3:D:14:DC:H2"	3:D:15:DC:H5"	1.61	0.83
1:A:368:GLU:HB2	1:A:427:LYS:HE3	1.66	0.77
2:B:394:ASP:HB2	2:B:519:LEU:HB3	1.67	0.77
1:A:76:GLN:H	1:A:76:GLN:NE2	1.83	0.76
2:B:787:ARG:HH11	2:B:787:ARG:CG	1.95	0.76
2:B:604:ASN:HA	2:B:607[B]:ARG:HG3	1.67	0.76
2:B:1004:PRO:O	2:B:1007:GLU:HG2	1.86	0.75
1:A:503:LEU:HD21	1:A:539:PHE:CE2	2.22	0.75
3:D:11:DA:H4'	3:D:12:DA:OP1	1.84	0.75
1:A:639:HIS:HB3	1:A:642:VAL:HG12	1.69	0.74
1:A:681:GLN:O	1:A:685:ILE:HG12	1.87	0.74
4:E:28:DA:H2"	4:E:29:DT:H5"	1.70	0.74
2:B:679:ILE:HD11	2:B:801:PHE:HE1	1.54	0.73
1:A:891:VAL:HG21	2:B:1101:LEU:HD21	1.71	0.73
4:E:48:DA:H5'	4:E:48:DA:H8	1.54	0.72
1:A:590:GLU:HB3	1:A:591:PRO:HD3	1.71	0.72
1:A:242:ASN:HD21	1:A:255:SER:H	1.37	0.72
2:B:746:GLU:HG2	2:B:768:VAL:HG21	1.70	0.72
2:B:725:ARG:HD3	2:B:731:PRO:HA	1.71	0.72
1:A:20:VAL:HG21	1:A:68:GLY:HA2	1.72	0.71
1:A:832:GLU:HG2	1:A:841:ILE:HD13	1.73	0.70
2:B:765:THR:HG22	2:B:767:ALA:H	1.55	0.70
2:B:340:LYS:HE3	2:B:345:VAL:HG22	1.74	0.70
2:B:498:ILE:HG12	2:B:510:LEU:HD13	1.75	0.69
1:A:807:THR:HB	1:A:810:THR:HB	1.72	0.69
2:B:787:ARG:HG2	2:B:787:ARG:NH1	1.94	0.69
4:E:26:DT:H2"	4:E:27:DC:H5'	1.75	0.69
1:A:242:ASN:ND2	1:A:255:SER:H	1.91	0.68
1:A:685:ILE:HD12	1:A:696:PRO:HD2	1.76	0.68
1:A:337:GLN:HG2	1:A:596:ASN:OD1	1.95	0.67
1:A:541:THR:HG22	1:A:551:PHE:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:40[A]:DC:H2"	4:E:41:DT:H5"	1.76	0.66
1:A:47:GLY:HA2	1:A:76:GLN:NE2	2.12	0.65
2:B:646:ILE:HG22	2:B:650:VAL:HG23	1.77	0.65
4:E:48:DA:H5'	4:E:48:DA:C8	2.31	0.65
1:A:521:TYR:H	1:A:560:ASN:HD21	1.43	0.64
2:B:447:GLU:HG2	2:B:500:TYR:CE1	2.32	0.64
2:B:569:LYS:O	2:B:573:GLN:HG2	1.97	0.64
2:B:691:THR:HA	2:B:794:CYS:SG	2.38	0.64
1:A:76:GLN:HE21	1:A:76:GLN:N	1.92	0.63
1:A:764:TRP:CE2	2:B:1080:LYS:HE3	2.33	0.63
2:B:836:ASP:HB2	2:B:854:ARG:NH1	2.14	0.63
1:A:577:ILE:O	1:A:581:ILE:HG12	1.97	0.63
2:B:612:ILE:HG21	2:B:636:LEU:HD21	1.81	0.63
1:A:128:LEU:HD13	1:A:134:ILE:HG22	1.81	0.62
1:A:414:LEU:N	1:A:415:PRO:HD2	2.14	0.62
1:A:633:ILE:HG13	1:A:701:GLU:HB2	1.82	0.62
1:A:706:ASP:HB2	1:A:742:ASP:HB2	1.81	0.62
1:A:243:ARG:HD3	1:A:286:PHE:HE1	1.64	0.62
1:A:425:GLU:O	1:A:430:LYS:HG3	1.99	0.61
2:B:433:ARG:O	2:B:437:VAL:HG23	2.01	0.61
2:B:893:LYS:O	2:B:897:ILE:HG12	2.01	0.60
4:E:36:DA:H2"	4:E:37:DC:OP2	1.99	0.60
1:A:801:HIS:CD2	1:A:822:CYS:HB3	2.37	0.60
1:A:427:LYS:HB3	1:A:427:LYS:HZ3	1.67	0.60
1:A:811:LEU:HD12	1:A:829:HIS:HD2	1.67	0.60
1:A:825:SER:HB3	2:B:976:ASP:OD2	2.02	0.60
2:B:869:VAL:HG23	2:B:870:PRO:HD2	1.83	0.60
2:B:747:ILE:HD11	2:B:771:PHE:HE2	1.67	0.59
1:A:162:GLY:HA3	1:A:265:VAL:HG12	1.84	0.59
1:A:438:THR:HB	1:A:439:PRO:HD3	1.83	0.59
2:B:392:VAL:HG11	2:B:519:LEU:HD13	1.84	0.58
1:A:895:PRO:O	1:A:899:MET:HG3	2.04	0.58
2:B:1058:SER:HB3	2:B:1061:LEU:HD12	1.84	0.58
2:B:858:ILE:HG23	2:B:862:LEU:HD12	1.86	0.58
1:A:481:LEU:HD23	1:A:570:TYR:HA	1.85	0.58
2:B:530:GLY:O	2:B:534:ARG:HD3	2.04	0.58
2:B:881[A]:ARG:NH1	2:B:1015:GLN:HG3	2.18	0.58
1:A:61:GLN:HG3	1:A:64:ILE:HD12	1.85	0.58
1:A:916:ILE:HD11	2:B:1102:TRP:HZ2	1.69	0.58
2:B:347:VAL:HG12	2:B:348:ASP:H	1.69	0.57
1:A:539:PHE:HE1	1:A:553:ASN:ND2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:LEU:HG	2:B:335:VAL:HG11	1.84	0.57
1:A:916:ILE:HD11	2:B:1102:TRP:CZ2	2.40	0.57
2:B:265:CYS:HA	2:B:273:THR:O	2.05	0.57
2:B:923:VAL:HG13	2:B:960:GLN:O	2.05	0.57
4:E:44:DA:H2"	4:E:45:DG:C8	2.40	0.57
2:B:568:LYS:O	2:B:572:THR:HG23	2.05	0.56
1:A:351:MET:O	1:A:704:ILE:HD13	2.05	0.56
1:A:539:PHE:HE1	1:A:553:ASN:HD21	1.52	0.56
2:B:351:MET:H	2:B:351:MET:CE	2.17	0.56
3:D:16:DG:H2'	3:D:17:DA:C8	2.40	0.56
2:B:784:ASN:HD22	2:B:787:ARG:HD2	1.69	0.56
1:A:562:GLU:HA	1:A:565:LYS:HB3	1.86	0.56
1:A:838:LYS:O	1:A:842:GLU:HG2	2.06	0.56
2:B:990:ARG:HG3	2:B:991:ASP:OD1	2.06	0.56
1:A:564:THR:O	1:A:568:THR:HG22	2.06	0.56
1:A:521:TYR:N	1:A:560:ASN:HD21	2.03	0.56
2:B:555:LEU:HA	2:B:831:VAL:HG21	1.88	0.56
2:B:784:ASN:HA	2:B:787:ARG:HD2	1.88	0.56
4:E:28:DA:C2'	4:E:29:DT:H5"	2.36	0.56
2:B:845:GLU:O	2:B:921:GLY:HA3	2.06	0.55
1:A:557:THR:O	1:A:561:GLU:HG3	2.06	0.55
2:B:277:PRO:HG2	2:B:280:ARG:HG3	1.88	0.55
1:A:630:GLY:HA2	1:A:777:PHE:HZ	1.72	0.55
2:B:755:ILE:HD12	2:B:756:PRO:O	2.06	0.55
1:A:676:SER:HB3	1:A:680:ARG:NH2	2.22	0.55
1:A:165:TYR:CZ	1:A:174:GLY:HA3	2.42	0.55
1:A:485:MET:O	1:A:489:GLU:HG3	2.08	0.54
1:A:408:TYR:HA	1:A:451:GLN:HE22	1.71	0.54
2:B:302:GLU:OE2	2:B:307:LYS:HE2	2.07	0.54
2:B:942:THR:HG23	2:B:945:GLU:H	1.72	0.54
2:B:1022:GLY:HA2	2:B:1059:TYR:OH	2.08	0.54
2:B:890[A]:MET:HE1	2:B:1048:TYR:HB3	1.88	0.54
2:B:671:SER:OG	2:B:672:PRO:HD3	2.08	0.54
1:A:435:VAL:O	1:A:439:PRO:HG2	2.08	0.54
2:B:961:SER:O	2:B:994:SER:HB2	2.08	0.54
4:E:47:DT:H1'	4:E:48:DA:H5"	1.90	0.54
2:B:219:ILE:HD13	2:B:219:ILE:H	1.72	0.54
2:B:985:LEU:O	2:B:989:ILE:HG13	2.08	0.54
2:B:746:GLU:HG2	2:B:768:VAL:CG2	2.38	0.54
2:B:865:GLN:HE21	2:B:868:TYR:N	1.98	0.54
2:B:1101:LEU:HA	2:B:1104:MET:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ILE:O	1:A:651:ILE:HG13	2.08	0.53
1:A:743:SER:O	1:A:776:ALA:HB1	2.09	0.53
2:B:494:LEU:O	2:B:498:ILE:HG13	2.09	0.53
2:B:501:LEU:HD21	2:B:509:MET:HE3	1.90	0.53
1:A:29:LYS:HB3	1:A:35:ARG:CZ	2.38	0.53
2:B:539:LEU:HD21	2:B:572:THR:HG22	1.89	0.53
1:A:243:ARG:HD3	1:A:286:PHE:CE1	2.43	0.53
1:A:639:HIS:HB3	1:A:642:VAL:CG1	2.38	0.53
1:A:756:THR:HG21	2:B:1002:TYR:HE1	1.72	0.53
1:A:477:ASN:O	1:A:481:LEU:HD13	2.08	0.53
1:A:527:CYS:HA	1:A:530:GLU:HB3	1.90	0.53
2:B:855:HIS:CG	2:B:858:ILE:HD13	2.45	0.52
1:A:210:MET:O	1:A:214:ARG:HG3	2.09	0.52
1:A:171:ARG:HH22	1:A:392:LYS:NZ	2.08	0.52
1:A:756:THR:HG21	2:B:1002:TYR:CE1	2.45	0.52
2:B:422:ALA:H	2:B:451:ASN:HD21	1.57	0.52
2:B:865:GLN:NE2	2:B:868:TYR:H	1.97	0.52
2:B:973[B]:SER:OG	2:B:976:ASP:HB2	2.09	0.52
1:A:211:GLY:O	1:A:215:GLN:HG2	2.10	0.52
1:A:212:LYS:O	1:A:216:ILE:HG12	2.10	0.51
1:A:632:ILE:HB	1:A:657:PHE:HB2	1.92	0.51
2:B:338:LEU:HD11	2:B:627:GLN:HB2	1.93	0.51
2:B:577:LYS:NZ	2:B:577:LYS:HA	2.25	0.51
4:E:28:DA:H2"	4:E:29:DT:C5'	2.40	0.51
1:A:362:LEU:HD22	1:A:436:PHE:HE2	1.76	0.51
2:B:781:ARG:O	2:B:785:GLN:HG3	2.10	0.51
3:D:13:DG:H2"	3:D:14:DC:C6	2.46	0.51
3:D:19:DC:H2"	3:D:20:DG:C8	2.45	0.51
1:A:400:ASN:OD1	1:A:402:GLN:HB3	2.11	0.51
1:A:769:TYR:CE2	1:A:773:LYS:HG2	2.46	0.51
2:B:598:VAL:HG22	2:B:649:ALA:HB1	1.93	0.51
2:B:312:ASN:HD22	2:B:312:ASN:H	1.59	0.51
2:B:512:LYS:HE2	2:B:810:HIS:CE1	2.45	0.51
2:B:885:ILE:HD12	2:B:897:ILE:HD11	1.92	0.51
3:D:15:DC:H6	3:D:15:DC:H5'	1.76	0.51
1:A:588:TYR:C	1:A:591:PRO:HD2	2.31	0.51
1:A:124:SER:HB2	1:A:125:PRO:HD2	1.92	0.50
2:B:331:ILE:HD11	2:B:387:ALA:HA	1.93	0.50
2:B:843:GLN:O	2:B:922:ILE:HG13	2.11	0.50
3:D:22:DT:H2'	3:D:23:DG:C8	2.47	0.50
1:A:450:PHE:HD2	1:A:451:GLN:HE21	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ILE:HD11	2:B:355:SER:C	2.31	0.50
1:A:514:ASP:HB2	1:A:522:TYR:CE1	2.46	0.50
2:B:559:LYS:HD3	2:B:607[B]:ARG:HA	1.93	0.50
1:A:678:TYR:O	1:A:681:GLN:HG2	2.12	0.50
1:A:740:THR:O	1:A:776:ALA:HB2	2.12	0.50
1:A:171:ARG:HH22	1:A:392:LYS:HZ2	1.60	0.50
1:A:673:GLY:O	1:A:802:VAL:HG21	2.12	0.50
2:B:832:ALA:HB1	2:B:912:TYR:CD1	2.47	0.50
1:A:375:THR:O	1:A:379:ASP:HB2	2.11	0.50
1:A:471:LYS:HE3	1:A:473:SER:OG	2.12	0.50
2:B:828:LEU:HD22	2:B:911:SER:HB2	1.94	0.49
1:A:550:LYS:N	1:A:550:LYS:HD2	2.27	0.49
2:B:846:ARG:HG2	2:B:960:GLN:HA	1.93	0.49
1:A:925:GLU:O	1:A:929:ARG:HG3	2.11	0.49
2:B:784:ASN:HD22	2:B:787:ARG:CD	2.25	0.49
1:A:383:ARG:HD3	1:A:413:GLN:NE2	2.28	0.49
1:A:745:ILE:O	1:A:778:CYS:HA	2.12	0.49
1:A:534:ARG:H	1:A:534:ARG:HD2	1.78	0.49
2:B:747:ILE:HD12	2:B:747:ILE:O	2.13	0.49
2:B:1104:MET:HB3	2:B:1109:ASP:HB3	1.94	0.49
1:A:684:VAL:O	1:A:688:MET:HG3	2.13	0.49
2:B:413:GLN:N	2:B:414:PRO:HD3	2.28	0.49
2:B:703:ILE:O	2:B:707:LYS:HG3	2.13	0.49
2:B:380:GLY:HA3	2:B:489:PRO:HB2	1.95	0.49
1:A:855:GLN:O	1:A:856:TYR:C	2.51	0.49
1:A:391:ALA:HB1	1:A:589:VAL:HG13	1.95	0.48
2:B:596:SER:HB2	2:B:598:VAL:HG23	1.95	0.48
2:B:986:GLU:HG2	2:B:990:ARG:NH1	2.29	0.48
1:A:32:THR:HG22	1:A:98:TYR:CE2	2.49	0.48
2:B:248:ARG:HH11	2:B:248:ARG:HB3	1.78	0.48
2:B:287:ARG:O	2:B:291:LYS:HG2	2.14	0.48
1:A:353:LYS:O	1:A:357:GLU:HG2	2.14	0.48
1:A:462:GLN:HA	1:A:465:ASN:HD22	1.78	0.48
1:A:625:LEU:HD22	1:A:631:ARG:HB2	1.96	0.48
2:B:721:LEU:O	2:B:725:ARG:HG3	2.13	0.48
2:B:880:GLU:OE2	2:B:1017:GLY:HA3	2.14	0.48
1:A:525:VAL:HB	1:A:551:PHE:CE2	2.49	0.48
2:B:736:VAL:HG22	2:B:744:MET:O	2.14	0.48
2:B:1093:LYS:HE3	2:B:1120:GLU:HG2	1.96	0.48
1:A:180:ASP:CG	1:A:186:ASN:HB2	2.35	0.48
2:B:851:LYS:HB2	2:B:917:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1060:GLY:O	2:B:1063:VAL:HG22	2.13	0.48
1:A:534:ARG:H	1:A:534:ARG:CD	2.27	0.47
2:B:604:ASN:HA	2:B:607[A]:ARG:HD3	1.95	0.47
2:B:1096:LYS:O	2:B:1100:LYS:HG3	2.14	0.47
1:A:346:ILE:HA	1:A:691:ILE:HD11	1.95	0.47
1:A:411:ILE:HG23	1:A:414:LEU:HD22	1.96	0.47
1:A:788:THR:HG22	1:A:799:ASN:HD21	1.78	0.47
2:B:305:ALA:HB3	2:B:788:GLU:CD	2.34	0.47
3:D:12:DA:H1'	3:D:13:DG:C8	2.49	0.47
1:A:525:VAL:HB	1:A:551:PHE:HE2	1.80	0.47
2:B:808:HIS:O	2:B:812:LEU:HG	2.15	0.47
3:D:13:DG:H2"	3:D:14:DC:C5	2.50	0.47
2:B:347:VAL:HG12	2:B:348:ASP:N	2.30	0.47
1:A:204:GLY:HA2	1:A:205:GLU:HA	1.60	0.47
1:A:574:GLN:O	1:A:578:VAL:HG23	2.15	0.47
1:A:780:PHE:CD1	1:A:780:PHE:C	2.88	0.47
2:B:621:HIS:O	2:B:623:LYS:HG3	2.14	0.47
2:B:849:VAL:HA	2:B:873:THR:O	2.15	0.47
1:A:563:TYR:O	1:A:567:LYS:HB2	2.15	0.47
1:A:814:LEU:O	1:A:815:TYR:HB2	2.14	0.47
2:B:223:LEU:HB3	3:D:18:DT:OP1	2.14	0.47
2:B:787:ARG:CG	2:B:787:ARG:NH1	2.64	0.47
1:A:630:GLY:HA2	1:A:777:PHE:CZ	2.50	0.47
2:B:512:LYS:N	2:B:513:PRO:HD3	2.30	0.47
2:B:497:ILE:HG22	2:B:510:LEU:HD11	1.97	0.47
1:A:359:ARG:HD2	1:A:691:ILE:O	2.15	0.46
2:B:339:ILE:HG12	2:B:346:ASN:O	2.15	0.46
2:B:376:ASN:ND2	2:B:397:GLN:HE21	2.12	0.46
2:B:679:ILE:HD11	2:B:801:PHE:CE1	2.43	0.46
1:A:532:VAL:O	1:A:532:VAL:HG12	2.15	0.46
1:A:194:ILE:HG22	1:A:196:PRO:HD3	1.96	0.46
2:B:488:LYS:HB2	2:B:489:PRO:HD3	1.96	0.46
2:B:1003:PRO:HB2	2:B:1004:PRO:HD3	1.98	0.46
2:B:316:LEU:HD11	3:D:17:DA:H3'	1.97	0.46
2:B:453:TYR:CD2	2:B:499:LYS:HD2	2.51	0.46
2:B:865:GLN:HE22	2:B:868:TYR:HD2	1.62	0.46
2:B:901:ALA:O	2:B:904:THR:HG22	2.16	0.46
1:A:391:ALA:HB2	1:A:592:MET:HG3	1.97	0.46
2:B:539:LEU:HD11	2:B:572:THR:HG22	1.97	0.46
1:A:165:TYR:CE2	1:A:174:GLY:HA3	2.51	0.45
1:A:407:LEU:O	1:A:411:ILE:HG12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLU:HG3	1:A:469:LEU:HG	1.97	0.45
1:A:481:LEU:HB3	1:A:570:TYR:HD1	1.80	0.45
2:B:954:ILE:HG23	2:B:987:TYR:CE2	2.51	0.45
4:E:31:DG:H5'	4:E:31:DG:C8	2.51	0.45
2:B:529[B]:ASN:OD1	2:B:531:THR:HB	2.15	0.45
2:B:865:GLN:NE2	2:B:868:TYR:HD2	2.15	0.45
2:B:881[A]:ARG:HH11	2:B:1015:GLN:HG3	1.79	0.45
1:A:55:ARG:O	1:A:59:LYS:HD3	2.16	0.45
2:B:351:MET:H	2:B:351:MET:HE3	1.81	0.45
3:D:6:DA:C8	3:D:7:DT:H72	2.52	0.45
1:A:283:ASP:HA	1:A:286:PHE:CD2	2.52	0.45
2:B:862:LEU:HD13	2:B:865:GLN:OE1	2.17	0.45
1:A:136:PHE:CG	1:A:389:ARG:HD2	2.52	0.45
2:B:455:GLU:OE1	2:B:457:SER:HB3	2.16	0.45
1:A:568:THR:O	1:A:572:GLU:HG2	2.17	0.45
2:B:404:GLU:OE2	2:B:956:LYS:HE2	2.17	0.45
1:A:22:PHE:CZ	1:A:117:TRP:HB2	2.52	0.45
1:A:642:VAL:HG23	1:A:645:GLN:HE21	1.81	0.45
2:B:378:PHE:HD2	2:B:489:PRO:HG2	1.81	0.45
2:B:765:THR:HG23	4:E:45:DG:OP2	2.17	0.45
2:B:890[A]:MET:CE	2:B:1021:MET:HB3	2.47	0.44
1:A:830:VAL:HG12	2:B:947:LEU:HD12	1.99	0.44
2:B:650:VAL:HG13	2:B:654:ILE:HD12	1.98	0.44
1:A:919:ASN:HA	1:A:924:ASN:HD21	1.82	0.44
2:B:576:LEU:O	2:B:922:ILE:HD13	2.18	0.44
2:B:986:GLU:HG2	2:B:990:ARG:HH11	1.82	0.44
1:A:803:THR:HG23	1:A:814:LEU:HD12	1.99	0.44
1:A:877:ARG:O	1:A:881:GLU:HG3	2.17	0.44
1:A:884:ILE:HG23	2:B:1098:PHE:CD1	2.52	0.44
2:B:1016:VAL:HG12	2:B:1017:GLY:N	2.31	0.44
1:A:145:ILE:CD1	1:A:165:TYR:HB2	2.48	0.44
1:A:492:MET:HE1	1:A:521:TYR:HB2	2.00	0.44
1:A:570:TYR:C	1:A:570:TYR:CD2	2.90	0.44
2:B:352:THR:HG21	2:B:415:VAL:HG11	2.00	0.44
2:B:423:LEU:HB2	2:B:428:GLU:OE1	2.18	0.44
2:B:218:SER:C	2:B:220:TYR:H	2.21	0.44
1:A:200:VAL:HB	1:A:227:ARG:HG3	1.98	0.44
1:A:368:GLU:CB	1:A:427:LYS:HE3	2.44	0.44
1:A:826:PHE:O	1:A:830:VAL:HG23	2.17	0.44
1:A:145:ILE:HG13	1:A:146:GLY:N	2.33	0.44
1:A:302:LEU:CD2	1:A:708:ILE:HB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:OE2	1:A:304:ILE:HG12	2.18	0.44
1:A:523:PHE:CE2	1:A:556:LEU:HD22	2.52	0.44
2:B:658:LEU:O	2:B:662:VAL:HG23	2.18	0.44
3:D:11:DA:H1'	3:D:12:DA:C8	2.53	0.44
2:B:949:ASP:O	2:B:953:ILE:HG13	2.18	0.43
1:A:496:LEU:HD22	1:A:513:LEU:HG	2.00	0.43
2:B:381:ILE:HD11	2:B:519:LEU:HD23	2.00	0.43
2:B:855:HIS:HB3	2:B:858:ILE:HB	1.98	0.43
1:A:359:ARG:O	1:A:363:VAL:HG23	2.17	0.43
1:A:503:LEU:HD22	1:A:503:LEU:N	2.33	0.43
1:A:831:ALA:O	1:A:836:PHE:HB2	2.18	0.43
2:B:378:PHE:CD2	2:B:489:PRO:HG2	2.53	0.43
2:B:642:GLU:O	2:B:646:ILE:HG13	2.18	0.43
1:A:530:GLU:HG2	2:B:761:LYS:NZ	2.33	0.43
1:A:254:ASN:O	1:A:257:VAL:HG22	2.19	0.43
1:A:651:ILE:HD11	1:A:815:TYR:C	2.39	0.43
1:A:783[B]:HIS:CD2	1:A:783[B]:HIS:H	2.36	0.43
1:A:154:ALA:HA	1:A:159:ARG:HA	2.01	0.43
2:B:286:ARG:HH11	2:B:335:VAL:HG13	1.84	0.43
1:A:607:SER:O	1:A:611:VAL:HG23	2.18	0.43
2:B:974:THR:O	2:B:978:ILE:HG13	2.19	0.43
1:A:220:GLY:HA2	1:A:304:ILE:HD12	1.99	0.43
1:A:234:THR:O	1:A:237:ILE:HG22	2.19	0.43
1:A:443:LEU:HD13	1:A:443:LEU:HA	1.90	0.43
1:A:552:THR:HB	1:A:556:LEU:HD23	2.01	0.43
1:A:922:PHE:O	1:A:926:ILE:HD12	2.19	0.43
2:B:890[A]:MET:HE1	2:B:892:GLY:HA3	2.00	0.43
2:B:512:LYS:HB3	2:B:512:LYS:HE3	1.85	0.43
2:B:590:GLU:O	2:B:594:SER:HB2	2.18	0.43
2:B:452:ILE:H	2:B:452:ILE:HD12	1.84	0.42
2:B:846:ARG:HA	2:B:921:GLY:O	2.19	0.42
2:B:923:VAL:HG12	2:B:925:GLY:H	1.83	0.42
1:A:579:LYS:NZ	1:A:579:LYS:HB3	2.34	0.42
2:B:438:SER:OG	2:B:443:ARG:HA	2.19	0.42
1:A:333:CYS:HB3	1:A:603:ASP:OD2	2.17	0.42
1:A:460:MET:O	1:A:463:VAL:HG12	2.19	0.42
2:B:452:ILE:HD12	2:B:452:ILE:N	2.34	0.42
2:B:650:VAL:HG21	2:B:663:ILE:HG21	2.02	0.42
1:A:284:SER:O	1:A:288:GLN:HG3	2.20	0.42
1:A:427:LYS:HB3	1:A:427:LYS:NZ	2.29	0.42
1:A:780:PHE:C	1:A:780:PHE:HD1	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:555:LEU:HA	2:B:831:VAL:CG2	2.49	0.42
1:A:213:LEU:O	1:A:217:ILE:HG13	2.19	0.42
2:B:647:ILE:HB	2:B:648:PRO:HD3	2.00	0.42
1:A:148:VAL:HG23	1:A:165:TYR:HB3	2.00	0.42
1:A:309:ALA:O	1:A:680:ARG:HD2	2.20	0.42
1:A:379:ASP:HA	1:A:382:ARG:NH1	2.34	0.42
1:A:639:HIS:CB	1:A:642:VAL:HG12	2.46	0.42
2:B:248:ARG:HB3	2:B:248:ARG:NH1	2.35	0.42
1:A:630:GLY:O	1:A:658:GLU:HA	2.20	0.42
2:B:531:THR:HA	2:B:534:ARG:NH1	2.35	0.42
2:B:978:ILE:HD13	2:B:1004:PRO:HG2	2.01	0.42
1:A:661:LYS:HB2	1:A:661:LYS:HE2	1.86	0.42
2:B:846:ARG:HA	2:B:921:GLY:C	2.40	0.42
2:B:755:ILE:HA	2:B:756:PRO:HD3	1.94	0.41
2:B:1019:TYR:CD2	2:B:1052:ARG:HA	2.55	0.41
1:A:750:LEU:HD21	1:A:766:ILE:HD12	2.02	0.41
2:B:279:HIS:CD2	2:B:280:ARG:HG2	2.55	0.41
1:A:484:ILE:O	1:A:488:LEU:HD13	2.20	0.41
1:A:679:ILE:HD12	1:A:746:ILE:HG23	2.00	0.41
1:A:724:THR:HG23	2:B:889:ASN:HB3	2.02	0.41
1:A:673:GLY:O	1:A:815:TYR:HD1	2.04	0.41
1:A:908:LEU:HD21	2:B:1110:LEU:HD11	2.03	0.41
2:B:814:LYS:HB3	2:B:814:LYS:HE2	1.78	0.41
2:B:836:ASP:HB2	2:B:854:ARG:HH12	1.83	0.41
1:A:61:GLN:HB3	2:B:339:ILE:CD1	2.51	0.41
1:A:337:GLN:HE21	1:A:337:GLN:HB2	1.62	0.41
1:A:493:GLN:O	1:A:497:ILE:HD13	2.21	0.41
1:A:566:ASN:HA	1:A:569:GLU:HG2	2.02	0.41
2:B:712:GLY:O	2:B:716:GLU:HG3	2.20	0.41
2:B:514:GLU:CD	2:B:514:GLU:H	2.24	0.41
2:B:655:GLN:C	2:B:660:ARG:HH12	2.24	0.41
3:D:12:DA:H4'	3:D:13:DG:OP1	2.20	0.41
1:A:709:LEU:HD12	1:A:739:ALA:HB2	2.03	0.41
1:A:753:GLY:HA2	2:B:889:ASN:ND2	2.36	0.41
1:A:920:ASN:OD1	1:A:922:PHE:HB3	2.20	0.41
1:A:615:ALA:HB1	1:A:616:PRO:HD2	2.03	0.41
1:A:634:LEU:HB2	1:A:655:VAL:HB	2.02	0.41
2:B:488:LYS:CB	2:B:489:PRO:HD3	2.51	0.41
2:B:615:GLY:O	2:B:619:ILE:HG13	2.19	0.41
2:B:633:VAL:HG13	2:B:677:LEU:HB2	2.03	0.41
2:B:882:VAL:HG11	2:B:985:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:NE2	1:A:299:TYR:HB2	2.36	0.41
1:A:352:ASP:OD2	1:A:354:ASN:HB2	2.19	0.41
1:A:374:GLN:HB3	1:A:378:GLU:OE1	2.21	0.41
1:A:821:VAL:HG22	1:A:822:CYS:N	2.35	0.41
1:A:849:LEU:HB3	1:A:929:ARG:NH1	2.36	0.41
2:B:283:VAL:HG12	2:B:287:ARG:HD2	2.03	0.41
2:B:449:MET:HG3	2:B:454:PHE:HE2	1.85	0.41
2:B:463:VAL:HG21	2:B:491:ILE:HG23	2.02	0.41
2:B:818:HIS:O	2:B:822:VAL:HG23	2.20	0.41
2:B:948:THR:O	2:B:952:GLU:HG3	2.21	0.41
1:A:401:LEU:HD23	1:A:468:PHE:O	2.21	0.41
2:B:392:VAL:HG13	2:B:519:LEU:HB2	2.03	0.40
2:B:581:ILE:HD13	2:B:908:GLN:HA	2.03	0.40
2:B:671:SER:N	2:B:672:PRO:CD	2.85	0.40
2:B:902:LEU:O	2:B:906:MET:HG3	2.21	0.40
1:A:616:PRO:HG2	1:A:643:GLU:HG2	2.03	0.40
2:B:604:ASN:HA	2:B:607[A]:ARG:CD	2.52	0.40
2:B:627:GLN:HE21	2:B:627:GLN:HB3	1.61	0.40
2:B:833:LYS:O	2:B:833:LYS:HG2	2.20	0.40
2:B:943:PHE:CE2	2:B:972:THR:HB	2.56	0.40
2:B:1087:LEU:HD23	2:B:1087:LEU:C	2.42	0.40
1:A:462:GLN:HB3	1:A:467:GLU:HB3	2.03	0.40
1:A:766:ILE:O	1:A:770:ILE:HG13	2.21	0.40
2:B:587:ALA:O	2:B:591:VAL:HG23	2.22	0.40
2:B:598:VAL:O	2:B:602:ILE:HG13	2.21	0.40
2:B:630:PHE:CZ	2:B:682:GLU:HG3	2.56	0.40
2:B:832:ALA:HB2	2:B:912:TYR:HB2	2.03	0.40
1:A:376:LEU:HD23	1:A:380:LEU:HD12	2.03	0.40
1:A:579:LYS:O	1:A:579:LYS:HD2	2.21	0.40
2:B:456:TYR:CE1	2:B:488:LYS:HG3	2.56	0.40
2:B:526:MET:HG3	2:B:925:GLY:HA2	2.03	0.40
2:B:942:THR:HG22	2:B:945:GLU:HG3	2.03	0.40
1:A:432:LEU:C	1:A:434:ALA:H	2.24	0.40
1:A:887:PHE:O	1:A:891:VAL:HG23	2.22	0.40
2:B:511:SER:O	2:B:512:LYS:HB2	2.22	0.40
2:B:905:ILE:O	2:B:909:ILE:HG13	2.21	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	855/934 (92%)	791 (92%)	62 (7%)	2 (0%)	47 73
2	B	848/918 (92%)	791 (93%)	56 (7%)	1 (0%)	51 78
All	All	1703/1852 (92%)	1582 (93%)	118 (7%)	3 (0%)	47 73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	644	VAL
2	B	1117	PHE
1	A	71	GLY

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	733/808 (91%)	711 (97%)	22 (3%)	41 70
2	B	752/818 (92%)	718 (96%)	34 (4%)	27 55
All	All	1485/1626 (91%)	1429 (96%)	56 (4%)	34 62

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	61	GLN
1	A	73	LYS

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Mol	Chain	Res	Type
1	A	76	GLN
1	A	148	VAL
1	A	223	LEU
1	A	337	GLN
1	A	377	GLN
1	A	428	HIS
1	A	458	LEU
1	A	464	GLU
1	A	525	VAL
1	A	569	GLU
1	A	579	LYS
1	A	610	HIS
1	A	617	VAL
1	A	638	ARG
1	A	724	THR
1	A	731	GLU
1	A	780	PHE
1	A	839	HIS
1	A	898	GLU
2	B	219	ILE
2	B	248	ARG
2	B	309	ILE
2	B	311	ASP
2	B	312	ASN
2	B	330	LEU
2	B	351	MET
2	B	376	ASN
2	B	450	ASP
2	B	487	GLU
2	B	529[A]	ASN
2	B	529[B]	ASN
2	B	533	LEU
2	B	534	ARG
2	B	542	GLN
2	B	543	THR
2	B	566	LYS
2	B	577	LYS
2	B	593	HIS
2	B	627	GLN
2	B	718	ARG
2	B	778	GLU
2	B	787	ARG

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Mol	Chain	Res	Type
2	B	845	GLU
2	B	846	ARG
2	B	866	ASP
2	B	869	VAL
2	B	878	ASP
2	B	890[A]	MET
2	B	890[B]	MET
2	B	929	ARG
2	B	970	ARG
2	B	1049	GLN
2	B	1095	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	76	GLN
1	A	239	GLN
1	A	242	ASN
1	A	377	GLN
1	A	409	GLN
1	A	419	GLN
1	A	428	HIS
1	A	451	GLN
1	A	465	ASN
1	A	536	ASN
1	A	553	ASN
1	A	560	ASN
1	A	574	GLN
1	A	785	HIS
1	A	816	GLN
1	A	829	HIS
1	A	846	GLN
1	A	855	GLN
1	A	924	ASN
2	B	262	ASN
2	B	312	ASN
2	B	376	ASN
2	B	458	HIS
2	B	461	GLN
2	B	582	ASN
2	B	604	ASN

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Mol	Chain	Res	Type
2	B	621	HIS
2	B	627	GLN
2	B	651	ASN
2	B	741	GLN
2	B	772	HIS
2	B	784	ASN
2	B	785	GLN
2	B	843	GLN
2	B	865	GLN
2	B	867	GLN
2	B	1049	GLN
2	B	1106	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	A	935	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)

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
5	ADP	A	935	-	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	935	ADP	C5-C4	2.57	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	935	ADP	C3'-C2'-C1'	3.63	106.44	100.98
5	A	935	ADP	PA-O3A-PB	-3.60	120.48	132.83
5	A	935	ADP	N3-C2-N1	-3.11	123.82	128.68
5	A	935	ADP	C4-C5-N7	-2.62	106.67	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	935	ADP	C5'-O5'-PA-O1A
5	A	935	ADP	O4'-C4'-C5'-O5'
5	A	935	ADP	C3'-C4'-C5'-O5'
5	A	935	ADP	C5'-O5'-PA-O3A

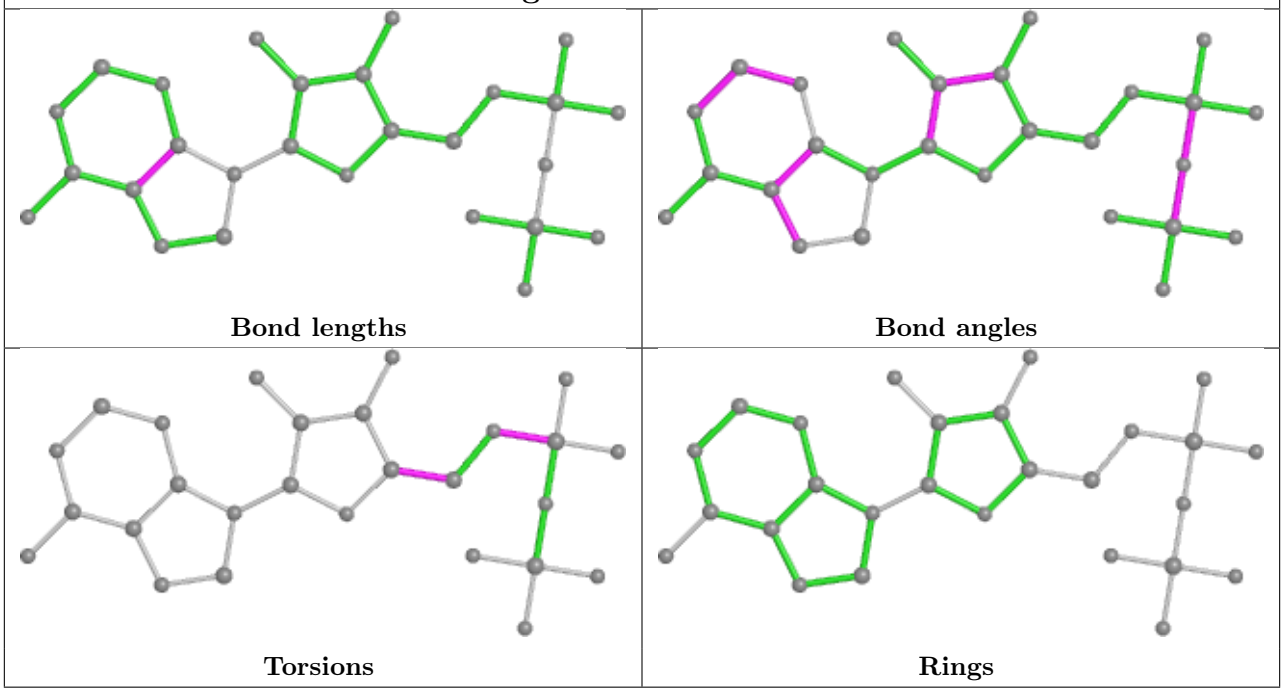
There are no ring outliers.

No monomer is involved in short contacts.

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 ADP A 935



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	868/934 (92%)	-0.01	36 (4%) 37 36	24, 67, 138, 256	0
2	B	852/918 (92%)	-0.20	16 (1%) 66 69	29, 58, 104, 190	0
3	D	21/24 (87%)	0.57	2 (9%) 8 6	58, 113, 170, 216	0
4	E	25/25 (100%)	0.80	3 (12%) 4 3	68, 119, 179, 188	0
All	All	1766/1901 (92%)	-0.08	57 (3%) 47 48	24, 63, 131, 256	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	THR	7.6
1	A	526	THR	6.6
1	A	70	ALA	6.0
1	A	534	ARG	5.5
3	D	3	DT	5.1
2	B	437	VAL	4.9
1	A	536	ASN	4.6
2	B	485	ASN	4.3
1	A	461	ASP	4.2
2	B	351	MET	4.1
1	A	527	CYS	4.0
1	A	525	VAL	4.0
2	B	1026	SER	3.9
1	A	206	THR	3.9
1	A	515	SER	3.9
1	A	531	LYS	3.9
1	A	543	ASP	3.8
2	B	218	SER	3.7
1	A	538	ASN	3.6
1	A	466	HIS	3.6
1	A	156	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	439	VAL	3.3
1	A	874	TYR	3.2
1	A	428	HIS	3.2
2	B	1044	VAL	3.2
2	B	438	SER	3.1
1	A	823	ASP	2.8
4	E	49	DG	2.8
1	A	822	CYS	2.7
4	E	36	DA	2.6
1	A	535	ASN	2.6
4	E	50	DG	2.5
1	A	548	GLY	2.5
3	D	4	DC	2.5
1	A	509	LYS	2.4
2	B	440	GLN	2.4
1	A	12	GLU	2.4
2	B	593	HIS	2.4
1	A	204	GLY	2.4
1	A	805	LEU	2.3
2	B	314	SER	2.3
1	A	505	LEU	2.2
1	A	112	SER	2.2
2	B	378	PHE	2.2
1	A	528	LYS	2.2
1	A	821	VAL	2.2
1	A	464	GLU	2.1
2	B	595	GLU	2.1
2	B	699	ASP	2.1
2	B	219	ILE	2.1
1	A	205	GLU	2.1
1	A	462	GLN	2.1
1	A	568	THR	2.1
1	A	74	ASN	2.0
2	B	348	ASP	2.0
1	A	873	CYS	2.0
1	A	529	GLU	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)

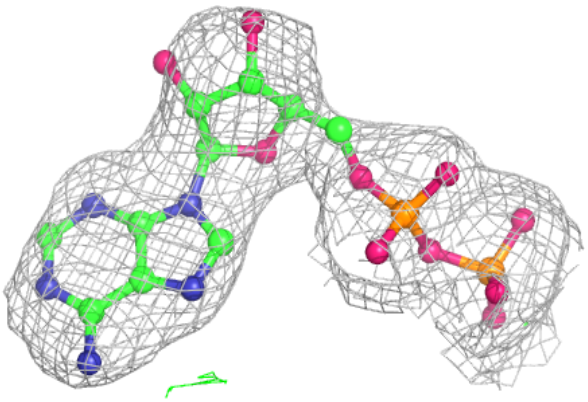
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

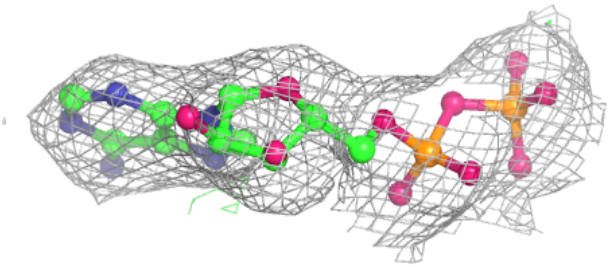
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	B	1	1/1	0.76	0.56	95,95,95,95	0
5	ADP	A	935	27/27	0.95	0.13	68,74,78,78	0

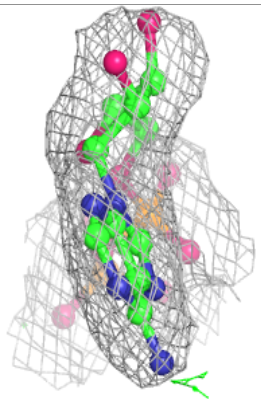
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 935:

$2mF_o$-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.