Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 05:28 AM EDT

PDB ID	:	5HV3
Title	:	Rifampin phosphotransferase G527Y mutant in complex with AMPPNP from Listeria monocytogenes
Authors	:	Zhang, P.; Qi, X.
Deposited on	:	2016-01-28
Resolution	:	3.12 Å(reported)

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

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

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

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

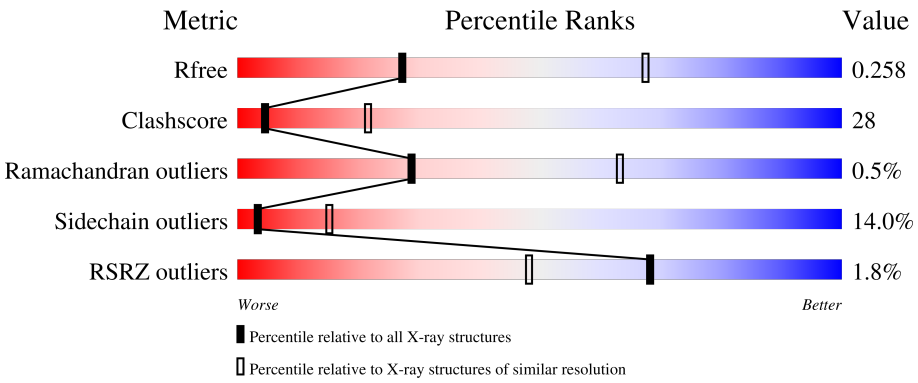
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.12 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	879	2% 51% 36% 8% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6691 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.

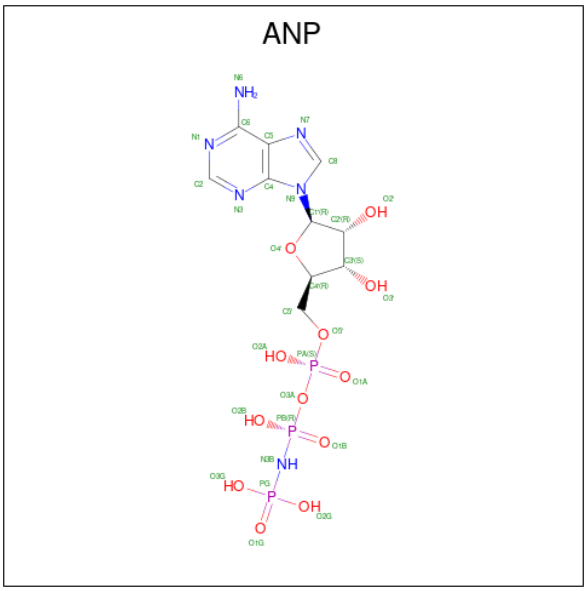
- Molecule 1 is a protein called Phosphoenolpyruvate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	846	6659	4227	1125	1277	30	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP A0A0S2YLC8
A	-10	ARG	-	expression tag	UNP A0A0S2YLC8
A	-9	GLY	-	expression tag	UNP A0A0S2YLC8
A	-8	SER	-	expression tag	UNP A0A0S2YLC8
A	-7	HIS	-	expression tag	UNP A0A0S2YLC8
A	-6	HIS	-	expression tag	UNP A0A0S2YLC8
A	-5	HIS	-	expression tag	UNP A0A0S2YLC8
A	-4	HIS	-	expression tag	UNP A0A0S2YLC8
A	-3	HIS	-	expression tag	UNP A0A0S2YLC8
A	-2	HIS	-	expression tag	UNP A0A0S2YLC8
A	-1	GLY	-	expression tag	UNP A0A0S2YLC8
A	0	SER	-	expression tag	UNP A0A0S2YLC8
A	527	TYR	GLY	engineered mutation	UNP A0A0S2YLC8

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	6	12	3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

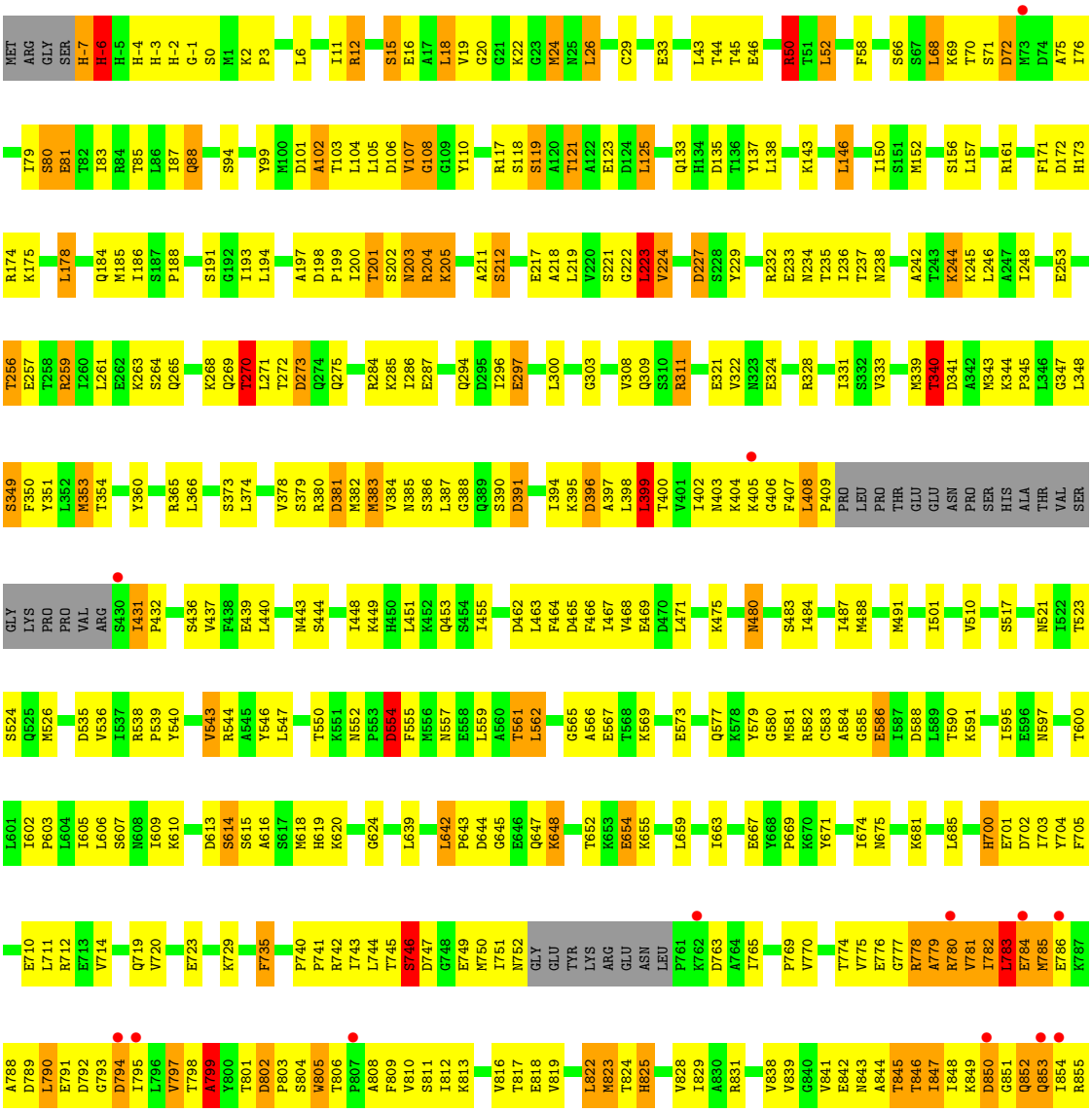
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

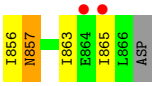
3 Residue-property plots (i)

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

- Molecule 1: Phosphoenolpyruvate synthase

Chain A: 2% 51% 36% 8%




I856
N857
I863
E864
I865
L866
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.69Å 127.99Å 140.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.51 – 3.12 34.51 – 3.12	Depositor EDS
% Data completeness (in resolution range)	88.2 (34.51-3.12) 88.3 (34.51-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.254 0.221 , 0.258	Depositor DCC
R_{free} test set	1821 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6691	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 (i)

5.1 Standard geometry (i)

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

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	0.71	0/6782	1.08	49/9173 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	197	ALA	CB-CA-C	22.01	143.12	110.10
1	A	735	PHE	C-N-CA	19.62	170.76	121.70
1	A	735	PHE	CB-CA-C	-19.48	71.45	110.40
1	A	735	PHE	N-CA-C	15.70	153.38	111.00
1	A	799	ALA	CB-CA-C	-14.09	88.97	110.10
1	A	-6	HIS	CB-CA-C	-13.86	82.69	110.40
1	A	431	ILE	N-CA-C	13.04	146.20	111.00
1	A	15	SER	N-CA-C	-12.13	78.24	111.00
1	A	431	ILE	CB-CA-C	-11.33	88.95	111.60
1	A	311	ARG	CB-CA-C	9.96	130.32	110.40
1	A	584	ALA	N-CA-C	-9.55	85.21	111.00
1	A	52	LEU	CB-CA-C	-9.35	92.44	110.20
1	A	340	THR	CB-CA-C	-9.16	86.88	111.60
1	A	554	ASP	N-CA-C	-9.04	86.59	111.00
1	A	197	ALA	N-CA-C	-8.71	87.48	111.00
1	A	852	GLN	N-CA-C	8.46	133.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	THR	CB-CA-C	-8.43	88.85	111.60
1	A	224	VAL	CB-CA-C	-8.25	95.73	111.40
1	A	799	ALA	N-CA-C	8.16	133.03	111.00
1	A	801	THR	N-CA-C	-8.09	89.16	111.00
1	A	567	GLU	N-CA-C	-7.92	89.62	111.00
1	A	794	ASP	N-CA-C	7.47	131.18	111.00
1	A	15	SER	C-N-CA	7.43	140.27	121.70
1	A	802	ASP	C-N-CD	-7.23	104.69	120.60
1	A	799	ALA	C-N-CA	7.01	139.22	121.70
1	A	238	ASN	CB-CA-C	6.84	124.08	110.40
1	A	108	GLY	N-CA-C	-6.68	96.39	113.10
1	A	801	THR	CB-CA-C	6.49	129.13	111.60
1	A	224	VAL	N-CA-C	6.45	128.41	111.00
1	A	852	GLN	CB-CA-C	-6.43	97.54	110.40
1	A	-7	HIS	C-N-CA	6.16	137.10	121.70
1	A	779	ALA	N-CA-C	6.16	127.62	111.00
1	A	50	ARG	CB-CA-C	-6.09	98.22	110.40
1	A	808	ALA	CB-CA-C	5.90	118.95	110.10
1	A	52	LEU	N-CA-C	5.89	126.92	111.00
1	A	102	ALA	CB-CA-C	-5.84	101.33	110.10
1	A	794	ASP	N-CA-CB	-5.81	100.15	110.60
1	A	270	THR	N-CA-C	5.65	126.26	111.00
1	A	223	LEU	C-N-CA	5.63	135.77	121.70
1	A	399	LEU	CA-CB-CG	-5.63	102.35	115.30
1	A	848	ILE	N-CA-C	-5.55	96.02	111.00
1	A	846	THR	N-CA-C	-5.51	96.13	111.00
1	A	11	ILE	CG1-CB-CG2	-5.49	99.33	111.40
1	A	585	GLY	N-CA-C	5.39	126.59	113.10
1	A	-6	HIS	N-CA-C	5.37	125.51	111.00
1	A	201	THR	CB-CA-C	-5.21	97.52	111.60
1	A	778	ARG	N-CA-C	5.21	125.06	111.00
1	A	783	LEU	N-CA-C	-5.04	97.38	111.00
1	A	171	PHE	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-6	HIS	Peptide
1	A	107	VAL	Peptide
1	A	15	SER	Peptide
1	A	340	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	554	ASP	Peptide
1	A	735	PHE	Peptide
1	A	799	ALA	Peptide

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	6659	0	6678	379	1
2	A	31	0	13	1	0
3	A	1	0	0	0	0
All	All	6691	0	6691	380	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 28.

All (380) 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:779:ALA:HB1	1:A:851:GLY:CA	1.53	1.37
1:A:431:ILE:CG2	1:A:431:ILE:O	1.63	1.33
1:A:799:ALA:O	1:A:819:VAL:HG13	1.16	1.31
1:A:779:ALA:CB	1:A:851:GLY:CA	2.07	1.30
1:A:779:ALA:HB2	1:A:851:GLY:C	1.52	1.28
1:A:779:ALA:CB	1:A:851:GLY:HA2	1.68	1.20
1:A:777:GLY:O	1:A:853:GLN:HB3	1.40	1.20
1:A:790:LEU:O	1:A:791:GLU:HG3	1.47	1.14
1:A:294:GLN:OE1	1:A:311:ARG:O	1.73	1.07
1:A:172:ASP:OD2	1:A:174:ARG:NH2	1.88	1.05
1:A:781:VAL:HG11	1:A:783:LEU:HD22	1.40	1.04
1:A:778:ARG:HB2	1:A:794:ASP:HB2	1.39	1.03
1:A:783:LEU:HD11	1:A:788:ALA:CB	1.89	1.03
1:A:841:VAL:HG21	1:A:844:ALA:HB2	1.40	1.02
1:A:778:ARG:HD2	1:A:794:ASP:HB3	1.34	1.02
1:A:843:ASN:O	1:A:846:THR:O	1.78	1.02
1:A:779:ALA:CB	1:A:851:GLY:C	2.28	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:LEU:HD12	1:A:784:GLU:N	1.79	0.97
1:A:780:ARG:NH2	1:A:845:THR:HB	1.79	0.97
1:A:52:LEU:O	1:A:58:PHE:CD2	2.17	0.97
1:A:799:ALA:O	1:A:819:VAL:CG1	2.12	0.96
1:A:781:VAL:HG12	1:A:783:LEU:HB2	1.45	0.95
1:A:779:ALA:HB1	1:A:851:GLY:HA2	0.96	0.95
1:A:780:ARG:HA	1:A:797:VAL:HG23	1.49	0.94
1:A:76:ILE:O	1:A:80:SER:OG	1.85	0.94
1:A:854:ILE:HD11	1:A:863:ILE:HG23	1.49	0.93
1:A:270:THR:HG22	1:A:270:THR:O	1.65	0.93
1:A:783:LEU:HD11	1:A:788:ALA:HB2	1.49	0.92
1:A:644:ASP:OD1	1:A:647:GLN:HB3	1.70	0.92
1:A:552:ASN:CG	1:A:554:ASP:O	2.09	0.92
1:A:217:GLU:O	1:A:221:SER:HB2	1.70	0.92
1:A:745:THR:HG22	1:A:747:ASP:H	1.34	0.91
1:A:340:THR:O	1:A:340:THR:OG1	1.75	0.90
1:A:778:ARG:HB2	1:A:794:ASP:CB	2.01	0.90
1:A:257:GLU:OE2	1:A:259:ARG:NH2	2.04	0.90
1:A:552:ASN:OD1	1:A:554:ASP:O	1.90	0.90
1:A:841:VAL:CG2	1:A:844:ALA:HB2	2.01	0.90
1:A:802:ASP:OD1	1:A:804:SER:OG	1.90	0.88
1:A:781:VAL:CG1	1:A:783:LEU:HB2	2.03	0.88
1:A:397:ALA:HB1	1:A:751:ILE:HG22	1.56	0.87
1:A:781:VAL:CG1	1:A:783:LEU:HD22	2.05	0.87
1:A:227:ASP:OD1	1:A:229:TYR:OH	1.93	0.86
1:A:777:GLY:O	1:A:853:GLN:CB	2.24	0.86
1:A:118:SER:HB2	1:A:178:LEU:HD21	1.59	0.85
1:A:201:THR:HG22	1:A:201:THR:O	1.74	0.83
1:A:72:ASP:O	1:A:76:ILE:HG13	1.77	0.83
1:A:198:ASP:OD2	1:A:199:PRO:HD2	1.78	0.83
1:A:779:ALA:HB2	1:A:851:GLY:O	1.78	0.82
1:A:781:VAL:CB	1:A:783:LEU:HB2	2.10	0.82
1:A:782:ILE:HG22	1:A:783:LEU:HA	1.61	0.81
1:A:107:VAL:O	1:A:184:GLN:NE2	2.11	0.81
1:A:790:LEU:O	1:A:791:GLU:CG	2.29	0.80
1:A:387:LEU:O	1:A:390:SER:O	2.01	0.79
1:A:779:ALA:HB1	1:A:851:GLY:HA3	1.58	0.77
1:A:852:GLN:C	1:A:853:GLN:HG3	2.02	0.77
1:A:802:ASP:HB2	1:A:803:PRO:HD3	1.66	0.77
1:A:818:GLU:OE2	1:A:845:THR:OG1	2.02	0.77
1:A:779:ALA:CB	1:A:851:GLY:HA3	2.11	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:ARG:CD	1:A:794:ASP:HB3	2.14	0.76
1:A:790:LEU:CA	1:A:791:GLU:OE2	2.32	0.76
1:A:224:VAL:CG1	1:A:246:LEU:HB2	2.16	0.75
1:A:242:ALA:O	1:A:244:LYS:NZ	2.20	0.75
1:A:253:GLU:N	1:A:253:GLU:OE1	2.19	0.75
1:A:785:MET:HA	1:A:788:ALA:HB2	1.69	0.75
1:A:792:ASP:OD1	1:A:793:GLY:N	2.20	0.74
1:A:270:THR:O	1:A:270:THR:CG2	2.35	0.74
1:A:431:ILE:O	1:A:431:ILE:HG22	0.82	0.74
1:A:-2:HIS:N	1:A:-1:GLY:HA3	2.03	0.73
1:A:22:LYS:HB3	1:A:119:SER:HB2	1.68	0.73
1:A:849:LYS:HD2	1:A:850:ASP:H	1.53	0.73
1:A:3:PRO:HG2	1:A:6:LEU:HD11	1.70	0.73
1:A:172:ASP:CG	1:A:174:ARG:HH21	1.93	0.72
1:A:852:GLN:O	1:A:853:GLN:HG3	1.88	0.72
1:A:790:LEU:C	1:A:791:GLU:CG	2.57	0.71
1:A:284:ARG:NH2	1:A:287:GLU:OE1	2.24	0.70
1:A:379:SER:HA	1:A:382:MET:HB3	1.72	0.70
1:A:44:THR:HG22	1:A:46:GLU:H	1.58	0.69
1:A:331:ILE:HD11	1:A:394:ILE:HG21	1.75	0.68
1:A:388:GLY:HA2	1:A:395:LYS:HD3	1.74	0.68
1:A:802:ASP:CB	1:A:803:PRO:CD	2.72	0.68
1:A:799:ALA:C	1:A:819:VAL:HG13	2.10	0.68
1:A:700:HIS:CD2	1:A:701:GLU:HG3	2.29	0.68
1:A:802:ASP:CG	1:A:803:PRO:HD2	2.14	0.67
1:A:391:ASP:HB3	1:A:394:ILE:HG13	1.76	0.67
1:A:203:ASN:O	1:A:203:ASN:ND2	2.25	0.67
1:A:783:LEU:HD11	1:A:788:ALA:HB1	1.72	0.66
1:A:224:VAL:HG11	1:A:246:LEU:O	1.95	0.66
1:A:790:LEU:C	1:A:791:GLU:OE2	2.34	0.66
1:A:20:GLY:HA2	1:A:121:THR:HG23	1.78	0.66
1:A:52:LEU:O	1:A:58:PHE:HD2	1.77	0.66
1:A:783:LEU:HD12	1:A:784:GLU:C	2.16	0.66
1:A:345:PRO:HD2	1:A:705:PHE:HA	1.79	0.65
1:A:224:VAL:HG12	1:A:246:LEU:HB2	1.77	0.65
1:A:642:LEU:CB	1:A:643:PRO:HD2	2.26	0.65
1:A:790:LEU:HA	1:A:791:GLU:OE2	1.95	0.65
1:A:198:ASP:OD2	1:A:199:PRO:CD	2.45	0.65
1:A:186:ILE:O	1:A:188:PRO:HD3	1.97	0.65
1:A:217:GLU:O	1:A:217:GLU:HG3	1.96	0.65
1:A:782:ILE:HG22	1:A:783:LEU:CA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:PHE:HB2	1:A:812:ILE:HD13	1.78	0.64
1:A:654:GLU:OE2	1:A:654:GLU:N	2.30	0.64
1:A:825:HIS:HD1	1:A:825:HIS:C	2.01	0.63
1:A:784:GLU:O	1:A:788:ALA:HB2	1.97	0.63
1:A:846:THR:O	1:A:847:ILE:HG22	1.98	0.63
1:A:789:ASP:O	1:A:791:GLU:OE2	2.17	0.62
1:A:781:VAL:HG12	1:A:783:LEU:CB	2.25	0.62
1:A:222:GLY:O	1:A:819:VAL:HG11	1.99	0.62
1:A:849:LYS:HD2	1:A:850:ASP:N	2.15	0.62
1:A:79:ILE:O	1:A:83:ILE:HG13	2.00	0.62
1:A:68:LEU:HD22	1:A:75:ALA:HB3	1.81	0.62
1:A:783:LEU:HD12	1:A:783:LEU:C	2.20	0.62
1:A:790:LEU:C	1:A:791:GLU:CD	2.59	0.62
1:A:749:GLU:HG2	1:A:751:ILE:HD11	1.81	0.61
1:A:-2:HIS:O	1:A:-2:HIS:ND1	2.33	0.61
1:A:397:ALA:HB2	1:A:752:ASN:HB3	1.83	0.61
1:A:809:PHE:O	1:A:812:ILE:HD13	2.01	0.61
1:A:806:THR:HA	1:A:809:PHE:HE2	1.65	0.61
1:A:544:ARG:HB3	1:A:544:ARG:CZ	2.31	0.61
1:A:841:VAL:HG11	1:A:863:ILE:HD12	1.82	0.61
1:A:552:ASN:ND2	1:A:554:ASP:O	2.33	0.60
1:A:790:LEU:HD11	1:A:812:ILE:HD11	1.84	0.60
1:A:199:PRO:HG2	1:A:822:LEU:HD21	1.82	0.60
1:A:365:ARG:HD3	1:A:740:PRO:HG3	1.84	0.60
1:A:557:ASN:HA	1:A:569:LYS:NZ	2.17	0.60
1:A:797:VAL:HA	1:A:816:VAL:O	2.02	0.59
1:A:223:LEU:O	1:A:223:LEU:HD23	2.02	0.59
1:A:381:ASP:O	1:A:385:ASN:ND2	2.31	0.59
1:A:431:ILE:O	1:A:432:PRO:O	2.20	0.59
1:A:235:THR:HG22	1:A:236:ILE:O	2.03	0.59
1:A:805:TRP:O	1:A:809:PHE:CD2	2.55	0.59
1:A:856:ILE:HG22	1:A:863:ILE:HG12	1.83	0.59
1:A:779:ALA:HB2	1:A:851:GLY:CA	1.94	0.59
1:A:344:LYS:HD2	1:A:704:TYR:HB3	1.83	0.58
1:A:223:LEU:HD23	1:A:223:LEU:N	2.18	0.58
1:A:487:ILE:HD11	1:A:669:PRO:HG2	1.85	0.58
1:A:642:LEU:HB2	1:A:643:PRO:HD2	1.85	0.58
1:A:172:ASP:HB3	1:A:175:LYS:HG3	1.84	0.58
1:A:201:THR:CG2	1:A:749:GLU:HG3	2.34	0.58
1:A:272:THR:O	1:A:275:GLN:N	2.37	0.58
1:A:782:ILE:CG2	1:A:783:LEU:HA	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASN:C	1:A:203:ASN:HD22	2.02	0.58
1:A:455:ILE:HG12	1:A:466:PHE:CE2	2.39	0.58
1:A:841:VAL:HG21	1:A:844:ALA:CB	2.26	0.57
1:A:852:GLN:O	1:A:853:GLN:CG	2.52	0.57
1:A:193:ILE:HD11	1:A:219:LEU:HD22	1.86	0.57
1:A:300:LEU:CD1	1:A:303:GLY:O	2.53	0.57
1:A:805:TRP:N	1:A:805:TRP:CD1	2.72	0.57
1:A:394:ILE:HD13	1:A:742:ARG:HG2	1.87	0.57
1:A:780:ARG:CA	1:A:797:VAL:HG23	2.31	0.56
1:A:538:ARG:NH2	1:A:609:ILE:HA	2.20	0.56
1:A:540:TYR:O	1:A:543:VAL:HG23	2.06	0.56
1:A:785:MET:CA	1:A:788:ALA:HB2	2.35	0.56
1:A:157:LEU:HB2	1:A:178:LEU:HD13	1.88	0.56
1:A:471:LEU:O	1:A:475:LYS:HG3	2.06	0.56
1:A:803:PRO:N	1:A:825:HIS:HD2	2.03	0.56
1:A:573:GLU:O	1:A:577:GLN:HG2	2.06	0.55
1:A:778:ARG:HD2	1:A:794:ASP:CB	2.22	0.55
1:A:464:PHE:O	1:A:468:VAL:HG23	2.07	0.55
1:A:-7:HIS:HB3	1:A:-6:HIS:HB2	1.87	0.55
1:A:439:GLU:O	1:A:443:ASN:ND2	2.40	0.55
1:A:535:ASP:OD1	1:A:538:ARG:NH1	2.40	0.55
1:A:841:VAL:HG11	1:A:863:ILE:CD1	2.37	0.55
1:A:333:VAL:HG12	1:A:366:LEU:O	2.07	0.55
1:A:223:LEU:HD23	1:A:223:LEU:H	1.71	0.55
1:A:380:ARG:HD3	1:A:402:ILE:HD12	1.89	0.54
1:A:104:LEU:O	1:A:108:GLY:HA2	2.07	0.54
1:A:201:THR:O	1:A:201:THR:CG2	2.47	0.54
1:A:588:ASP:OD1	1:A:590:THR:OG1	2.19	0.54
1:A:782:ILE:CG2	1:A:783:LEU:CA	2.85	0.54
1:A:802:ASP:C	1:A:825:HIS:HD2	2.10	0.54
1:A:849:LYS:HG3	1:A:850:ASP:HB2	1.90	0.54
1:A:464:PHE:HE1	1:A:711:LEU:HG	1.72	0.54
1:A:782:ILE:N	1:A:783:LEU:HA	2.21	0.54
1:A:18:LEU:O	1:A:45:THR:HG23	2.07	0.54
1:A:16:GLU:HG3	1:A:24:MET:SD	2.48	0.54
1:A:780:ARG:HG2	1:A:781:VAL:N	2.22	0.54
1:A:781:VAL:HB	1:A:783:LEU:CB	2.37	0.54
1:A:81:GLU:O	1:A:85:THR:HG23	2.08	0.53
1:A:805:TRP:O	1:A:809:PHE:CE2	2.62	0.53
1:A:88:GLN:HE21	1:A:152:MET:HG2	1.72	0.53
1:A:465:ASP:OD1	1:A:712:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:H	1:A:244:LYS:HZ3	1.56	0.53
1:A:536:VAL:O	1:A:539:PRO:HD2	2.08	0.53
1:A:779:ALA:CB	1:A:851:GLY:O	2.47	0.53
1:A:781:VAL:CB	1:A:783:LEU:HD22	2.39	0.53
1:A:2:LYS:HB2	1:A:46:GLU:HG3	1.89	0.53
1:A:782:ILE:N	1:A:783:LEU:CA	2.72	0.53
1:A:781:VAL:HG12	1:A:783:LEU:HD13	1.91	0.53
1:A:404:LYS:O	1:A:406:GLY:N	2.39	0.53
1:A:583:CYS:O	1:A:586:GLU:HG3	2.10	0.52
1:A:123:GLU:O	1:A:125:LEU:HD12	2.08	0.52
1:A:223:LEU:N	1:A:223:LEU:CD2	2.72	0.52
1:A:648:LYS:O	1:A:652:THR:HG23	2.10	0.52
1:A:841:VAL:CG2	1:A:844:ALA:CB	2.82	0.52
1:A:451:LEU:O	1:A:455:ILE:HG13	2.10	0.52
1:A:212:SER:OG	1:A:219:LEU:HD12	2.10	0.52
1:A:269:GLN:HG2	1:A:271:LEU:O	2.09	0.52
1:A:544:ARG:HD3	1:A:610:LYS:NZ	2.25	0.52
1:A:351:TYR:CD2	1:A:366:LEU:HD13	2.45	0.51
1:A:583:CYS:H	1:A:586:GLU:HG2	1.75	0.51
1:A:227:ASP:OD1	1:A:229:TYR:CZ	2.63	0.51
1:A:269:GLN:NE2	1:A:273:ASP:OD2	2.42	0.51
1:A:749:GLU:HG2	1:A:751:ILE:CD1	2.40	0.51
1:A:803:PRO:HA	1:A:825:HIS:CD2	2.45	0.51
1:A:328:ARG:H	1:A:746:SER:HB3	1.76	0.51
2:A:901:ANP:H5'1	2:A:901:ANP:H8	1.92	0.51
1:A:642:LEU:HB3	1:A:643:PRO:HD2	1.93	0.51
1:A:224:VAL:HG13	1:A:246:LEU:HB2	1.90	0.51
1:A:781:VAL:HB	1:A:783:LEU:HB2	1.87	0.51
1:A:173:HIS:O	1:A:174:ARG:HB2	2.11	0.50
1:A:218:ALA:HB2	1:A:248:ILE:HD12	1.94	0.50
1:A:440:LEU:HD11	1:A:483:SER:HA	1.93	0.50
1:A:557:ASN:HA	1:A:569:LYS:HZ2	1.73	0.50
1:A:294:GLN:OE1	1:A:311:ARG:C	2.47	0.50
1:A:137:TYR:CZ	1:A:152:MET:HE2	2.46	0.50
1:A:273:ASP:OD2	1:A:273:ASP:N	2.44	0.50
1:A:565:GLY:O	1:A:566:ALA:HB3	2.12	0.50
1:A:822:LEU:HD23	1:A:823:MET:SD	2.51	0.50
1:A:333:VAL:HG22	1:A:333:VAL:O	2.11	0.50
1:A:449:LYS:O	1:A:453:GLN:HG3	2.12	0.50
1:A:803:PRO:HD2	1:A:804:SER:H	1.76	0.50
1:A:546:TYR:CE1	1:A:550:THR:HB	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:O	1:A:610:LYS:HG2	2.11	0.49
1:A:809:PHE:HZ	1:A:829:ILE:HG21	1.77	0.49
1:A:741:PRO:HG3	1:A:750:MET:HE2	1.94	0.49
1:A:300:LEU:HD11	1:A:303:GLY:O	2.13	0.49
1:A:642:LEU:CB	1:A:643:PRO:CD	2.89	0.49
1:A:615:SER:O	1:A:619:HIS:ND1	2.46	0.49
1:A:343:MET:HB3	1:A:348:LEU:HG	1.93	0.49
1:A:535:ASP:O	1:A:538:ARG:HG3	2.13	0.48
1:A:395:LYS:HG2	1:A:399:LEU:HD12	1.95	0.48
1:A:781:VAL:C	1:A:783:LEU:HB2	2.34	0.48
1:A:521:ASN:HB3	1:A:524:SER:HB3	1.95	0.48
1:A:194:LEU:HD22	1:A:296:ILE:HD12	1.96	0.48
1:A:350:PHE:HA	1:A:353:MET:HG3	1.95	0.48
1:A:805:TRP:O	1:A:809:PHE:HD2	1.97	0.48
1:A:790:LEU:HD13	1:A:811:SER:OG	2.14	0.48
1:A:157:LEU:HD13	1:A:178:LEU:HD12	1.96	0.48
1:A:383:MET:O	1:A:386:SER:N	2.43	0.47
1:A:103:THR:O	1:A:106:ASP:N	2.31	0.47
1:A:842:GLU:HG3	1:A:843:ASN:N	2.30	0.47
1:A:781:VAL:CG1	1:A:783:LEU:CD2	2.85	0.47
1:A:68:LEU:CD2	1:A:75:ALA:CB	2.92	0.47
1:A:710:GLU:O	1:A:714:VAL:HG23	2.14	0.47
1:A:802:ASP:O	1:A:804:SER:N	2.47	0.47
1:A:70:THR:HG22	1:A:70:THR:O	2.14	0.47
1:A:642:LEU:HB2	1:A:643:PRO:CD	2.40	0.47
1:A:841:VAL:HG23	1:A:844:ALA:HB2	1.92	0.47
1:A:198:ASP:CG	1:A:200:ILE:O	2.53	0.47
1:A:374:LEU:O	1:A:380:ARG:NH2	2.42	0.47
1:A:261:LEU:HD22	1:A:265:GLN:HG2	1.97	0.47
1:A:652:THR:O	1:A:655:LYS:HB2	2.15	0.47
1:A:780:ARG:HH22	1:A:845:THR:HB	1.75	0.47
1:A:806:THR:HA	1:A:809:PHE:CE2	2.47	0.47
1:A:-7:HIS:HB3	1:A:-6:HIS:CB	2.45	0.46
1:A:616:ALA:O	1:A:620:LYS:HB2	2.14	0.46
1:A:741:PRO:HD3	1:A:750:MET:HE1	1.97	0.46
1:A:349:SER:O	1:A:353:MET:HG2	2.16	0.46
1:A:775:VAL:HG21	1:A:813:LYS:O	2.15	0.46
1:A:265:GLN:OE1	1:A:265:GLN:HA	2.16	0.46
1:A:380:ARG:O	1:A:383:MET:HB3	2.16	0.46
1:A:396:ASP:OD2	1:A:396:ASP:N	2.48	0.46
1:A:354:THR:HA	1:A:475:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:O	1:A:121:THR:HG21	2.16	0.46
1:A:463:LEU:O	1:A:466:PHE:HB3	2.15	0.46
1:A:591:LYS:O	1:A:681:LYS:NZ	2.48	0.46
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.82	0.46
1:A:146:LEU:O	1:A:150:ILE:HG13	2.15	0.46
1:A:218:ALA:O	1:A:221:SER:HB3	2.16	0.46
1:A:802:ASP:HB2	1:A:803:PRO:CD	2.32	0.46
1:A:605:ILE:O	1:A:609:ILE:HG13	2.16	0.46
1:A:201:THR:O	1:A:202:SER:C	2.54	0.46
1:A:659:LEU:O	1:A:663:ILE:HB	2.16	0.46
1:A:339:MET:HG3	1:A:341:ASP:H	1.81	0.45
1:A:602:ILE:N	1:A:603:PRO:HD2	2.30	0.45
1:A:828:VAL:HG12	1:A:831:ARG:HH22	1.81	0.45
1:A:68:LEU:HD22	1:A:75:ALA:CB	2.45	0.45
1:A:580:GLY:HA3	1:A:595:ILE:HB	1.97	0.45
1:A:50:ARG:O	1:A:50:ARG:HG3	2.12	0.45
1:A:770:VAL:HG21	1:A:839:VAL:HG22	1.98	0.45
1:A:639:LEU:HD23	1:A:639:LEU:HA	1.81	0.45
1:A:774:THR:OG1	1:A:857:ASN:HB2	2.17	0.45
1:A:803:PRO:CD	1:A:804:SER:H	2.30	0.45
1:A:26:LEU:HD13	1:A:26:LEU:HA	1.73	0.45
1:A:825:HIS:C	1:A:825:HIS:ND1	2.62	0.45
1:A:193:ILE:HD11	1:A:219:LEU:CD2	2.46	0.45
1:A:244:LYS:HZ2	1:A:244:LYS:HG3	1.68	0.45
1:A:780:ARG:HH11	1:A:782:ILE:HA	1.82	0.45
1:A:781:VAL:C	1:A:783:LEU:CB	2.85	0.45
1:A:297:GLU:HB2	1:A:309:GLN:HB3	1.99	0.44
1:A:804:SER:OG	1:A:805:TRP:CD1	2.70	0.44
1:A:345:PRO:HD2	1:A:704:TYR:O	2.18	0.44
1:A:397:ALA:HB1	1:A:751:ILE:CG2	2.37	0.44
1:A:44:THR:HG22	1:A:46:GLU:N	2.30	0.44
1:A:268:LYS:HA	1:A:268:LYS:HD3	1.70	0.44
1:A:523:THR:OG1	1:A:667:GLU:HG2	2.18	0.44
1:A:742:ARG:HD2	1:A:752:ASN:ND2	2.33	0.44
1:A:444:SER:O	1:A:448:ILE:HG13	2.18	0.44
1:A:484:ILE:O	1:A:488:MET:HG2	2.17	0.44
1:A:816:VAL:HA	1:A:838:VAL:O	2.18	0.44
1:A:101:ASP:OD1	1:A:110:TYR:OH	2.23	0.44
1:A:854:ILE:HG12	1:A:855:ARG:N	2.32	0.44
1:A:464:PHE:CE1	1:A:711:LEU:HG	2.51	0.43
1:A:526:MET:HB2	1:A:579:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:PHE:CZ	1:A:602:ILE:HD11	2.53	0.43
1:A:822:LEU:O	1:A:822:LEU:HG	2.18	0.43
1:A:22:LYS:HB3	1:A:119:SER:CB	2.45	0.43
1:A:349:SER:O	1:A:353:MET:CG	2.66	0.43
1:A:378:VAL:O	1:A:382:MET:HB2	2.17	0.43
1:A:480:ASN:OD1	1:A:480:ASN:N	2.50	0.43
1:A:745:THR:HB	1:A:749:GLU:HB3	2.00	0.43
1:A:780:ARG:NH1	1:A:782:ILE:HD13	2.33	0.43
1:A:198:ASP:HA	1:A:199:PRO:HD3	1.60	0.43
1:A:135:ASP:H	1:A:156:SER:HB2	1.81	0.43
1:A:211:ALA:O	1:A:227:ASP:HB2	2.18	0.43
1:A:235:THR:O	1:A:237:THR:HG23	2.16	0.43
1:A:354:THR:HG22	1:A:471:LEU:HD22	2.01	0.43
1:A:517:SER:OG	1:A:624:GLY:HA3	2.19	0.43
1:A:561:THR:HG23	1:A:562:LEU:HG	2.01	0.43
1:A:173:HIS:C	1:A:175:LYS:H	2.22	0.43
1:A:805:TRP:H	1:A:805:TRP:HD1	1.66	0.43
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.90	0.43
1:A:778:ARG:CG	1:A:794:ASP:HB3	2.47	0.43
1:A:101:ASP:OD1	1:A:143:LYS:HD2	2.19	0.42
1:A:172:ASP:O	1:A:175:LYS:HB2	2.19	0.42
1:A:431:ILE:O	1:A:432:PRO:C	2.57	0.42
1:A:395:LYS:O	1:A:398:LEU:HB3	2.20	0.42
1:A:743:ILE:HB	1:A:751:ILE:HB	2.00	0.42
1:A:138:LEU:HD22	1:A:185:MET:HE1	2.01	0.42
1:A:347:GLY:HA3	1:A:588:ASP:OD1	2.20	0.42
1:A:809:PHE:CZ	1:A:829:ILE:HG21	2.54	0.42
1:A:286:ILE:HD12	1:A:296:ILE:HD13	2.01	0.42
1:A:802:ASP:C	1:A:825:HIS:CD2	2.91	0.42
1:A:597:ASN:ND2	1:A:600:THR:HG23	2.35	0.42
1:A:804:SER:OG	1:A:805:TRP:HD1	2.03	0.42
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.85	0.42
1:A:436:SER:OG	1:A:437:VAL:N	2.52	0.42
1:A:552:ASN:OD1	1:A:554:ASP:C	2.55	0.42
1:A:285:LYS:HB2	1:A:285:LYS:HE2	1.90	0.42
1:A:462:ASP:O	1:A:466:PHE:N	2.41	0.42
1:A:643:PRO:C	1:A:645:GLY:N	2.70	0.42
1:A:785:MET:HA	1:A:788:ALA:CB	2.46	0.42
1:A:809:PHE:O	1:A:810:VAL:C	2.56	0.42
1:A:781:VAL:HG11	1:A:783:LEU:CD2	2.29	0.42
1:A:405:LYS:HD3	1:A:405:LYS:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:ARG:CB	1:A:794:ASP:CB	2.86	0.41
1:A:322:VAL:HG22	1:A:360:TYR:CE1	2.55	0.41
1:A:702:ASP:OD1	1:A:729:LYS:NZ	2.29	0.41
1:A:765:ILE:HD12	1:A:863:ILE:HG22	2.01	0.41
1:A:19:VAL:O	1:A:119:SER:OG	2.38	0.41
1:A:248:ILE:CG2	1:A:256:THR:HG23	2.49	0.41
1:A:582:ARG:HG2	1:A:674:ILE:HD11	2.01	0.41
1:A:778:ARG:O	1:A:795:ILE:HG12	2.20	0.41
1:A:68:LEU:HD21	1:A:75:ALA:HB1	2.03	0.41
1:A:407:PHE:CZ	1:A:745:THR:HG23	2.55	0.41
1:A:781:VAL:CA	1:A:783:LEU:HB2	2.49	0.41
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.76	0.41
1:A:83:ILE:O	1:A:87:ILE:HG13	2.21	0.41
1:A:203:ASN:C	1:A:205:LYS:H	2.23	0.41
1:A:703:ILE:C	1:A:705:PHE:N	2.73	0.41
1:A:798:THR:HG22	1:A:799:ALA:H	1.86	0.41
1:A:263:LYS:O	1:A:264:SER:C	2.56	0.41
1:A:663:ILE:HD12	1:A:663:ILE:HA	1.87	0.41
1:A:781:VAL:CG1	1:A:783:LEU:HD13	2.50	0.41
1:A:805:TRP:N	1:A:805:TRP:HD1	2.16	0.41
1:A:744:LEU:HD13	1:A:750:MET:HE2	2.03	0.41
1:A:769:PRO:O	1:A:770:VAL:HB	2.20	0.41
1:A:783:LEU:CD1	1:A:784:GLU:C	2.85	0.41
1:A:248:ILE:HG23	1:A:256:THR:HG23	2.01	0.40
1:A:671:TYR:O	1:A:675:ASN:HB2	2.21	0.40
1:A:803:PRO:CA	1:A:825:HIS:HD2	2.33	0.40
1:A:-7:HIS:CB	1:A:-6:HIS:HB2	2.51	0.40
1:A:203:ASN:O	1:A:204:ARG:CB	2.70	0.40
1:A:408:LEU:HA	1:A:409:PRO:O	2.21	0.40
1:A:547:LEU:H	1:A:547:LEU:HG	1.77	0.40
1:A:782:ILE:CD1	1:A:782:ILE:O	2.70	0.40
1:A:99:TYR:O	1:A:102:ALA:HB3	2.21	0.40
1:A:203:ASN:O	1:A:747:ASP:O	2.39	0.40
1:A:501:ILE:HD12	1:A:510:VAL:HG11	2.04	0.40
1:A:798:THR:O	1:A:817:THR:HA	2.22	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)
1:A:324:GLU:OE2	1:A:614:SER:OG[1_455]	1.99	0.21

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	840/879 (96%)	746 (89%)	90 (11%)	4 (0%)	29 63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	847	ILE
1	A	270	THR
1	A	746	SER
1	A	12	ARG

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	726/757 (96%)	624 (86%)	102 (14%)	3 15

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	HIS
1	A	-4	HIS
1	A	-3	HIS
1	A	0	SER
1	A	12	ARG
1	A	18	LEU
1	A	24	MET

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	29	CYS
1	A	33	GLU
1	A	50	ARG
1	A	66	SER
1	A	68	LEU
1	A	69	LYS
1	A	71	SER
1	A	72	ASP
1	A	80	SER
1	A	81	GLU
1	A	88	GLN
1	A	94	SER
1	A	105	LEU
1	A	117	ARG
1	A	119	SER
1	A	121	THR
1	A	125	LEU
1	A	133	GLN
1	A	146	LEU
1	A	161	ARG
1	A	178	LEU
1	A	191	SER
1	A	203	ASN
1	A	204	ARG
1	A	205	LYS
1	A	212	SER
1	A	223	LEU
1	A	227	ASP
1	A	232	ARG
1	A	233	GLU
1	A	234	ASN
1	A	244	LYS
1	A	245	LYS
1	A	256	THR
1	A	259	ARG
1	A	273	ASP
1	A	297	GLU
1	A	308	VAL
1	A	321	GLU
1	A	349	SER
1	A	353	MET

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Mol	Chain	Res	Type
1	A	373	SER
1	A	381	ASP
1	A	383	MET
1	A	384	VAL
1	A	391	ASP
1	A	396	ASP
1	A	399	LEU
1	A	400	THR
1	A	403	ASN
1	A	408	LEU
1	A	467	ILE
1	A	469	GLU
1	A	480	ASN
1	A	491	MET
1	A	543	VAL
1	A	559	LEU
1	A	561	THR
1	A	562	LEU
1	A	581	MET
1	A	586	GLU
1	A	607	SER
1	A	613	ASP
1	A	614	SER
1	A	618	MET
1	A	642	LEU
1	A	648	LYS
1	A	654	GLU
1	A	700	HIS
1	A	719	GLN
1	A	720	VAL
1	A	723	GLU
1	A	746	SER
1	A	763	ASP
1	A	776	GLU
1	A	780	ARG
1	A	781	VAL
1	A	782	ILE
1	A	783	LEU
1	A	784	GLU
1	A	785	MET
1	A	786	GLU
1	A	790	LEU

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Mol	Chain	Res	Type
1	A	797	VAL
1	A	805	TRP
1	A	822	LEU
1	A	823	MET
1	A	824	THR
1	A	825	HIS
1	A	845	THR
1	A	850	ASP
1	A	853	GLN
1	A	857	ASN
1	A	865	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	139	ASN
1	A	752	ASN
1	A	825	HIS

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	$\#\|Z\| > 2$
2	ANP	A	901	3	29,33,33	1.18	3 (10%)	31,52,52	1.34	3 (9%)

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	ANP	A	901	3	-	5/14/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ANP	PG-N3B	3.04	1.71	1.63
2	A	901	ANP	PB-O1B	2.73	1.50	1.46
2	A	901	ANP	PB-N3B	2.31	1.69	1.63

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	ANP	PB-O3A-PA	-5.15	114.50	132.62
2	A	901	ANP	O3G-PG-O1G	-2.09	108.19	113.45
2	A	901	ANP	O2B-PB-O3A	2.02	111.37	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ANP	PG-N3B-PB-O1B
2	A	901	ANP	C5'-O5'-PA-O1A
2	A	901	ANP	C5'-O5'-PA-O3A
2	A	901	ANP	C5'-O5'-PA-O2A
2	A	901	ANP	O4'-C4'-C5'-O5'

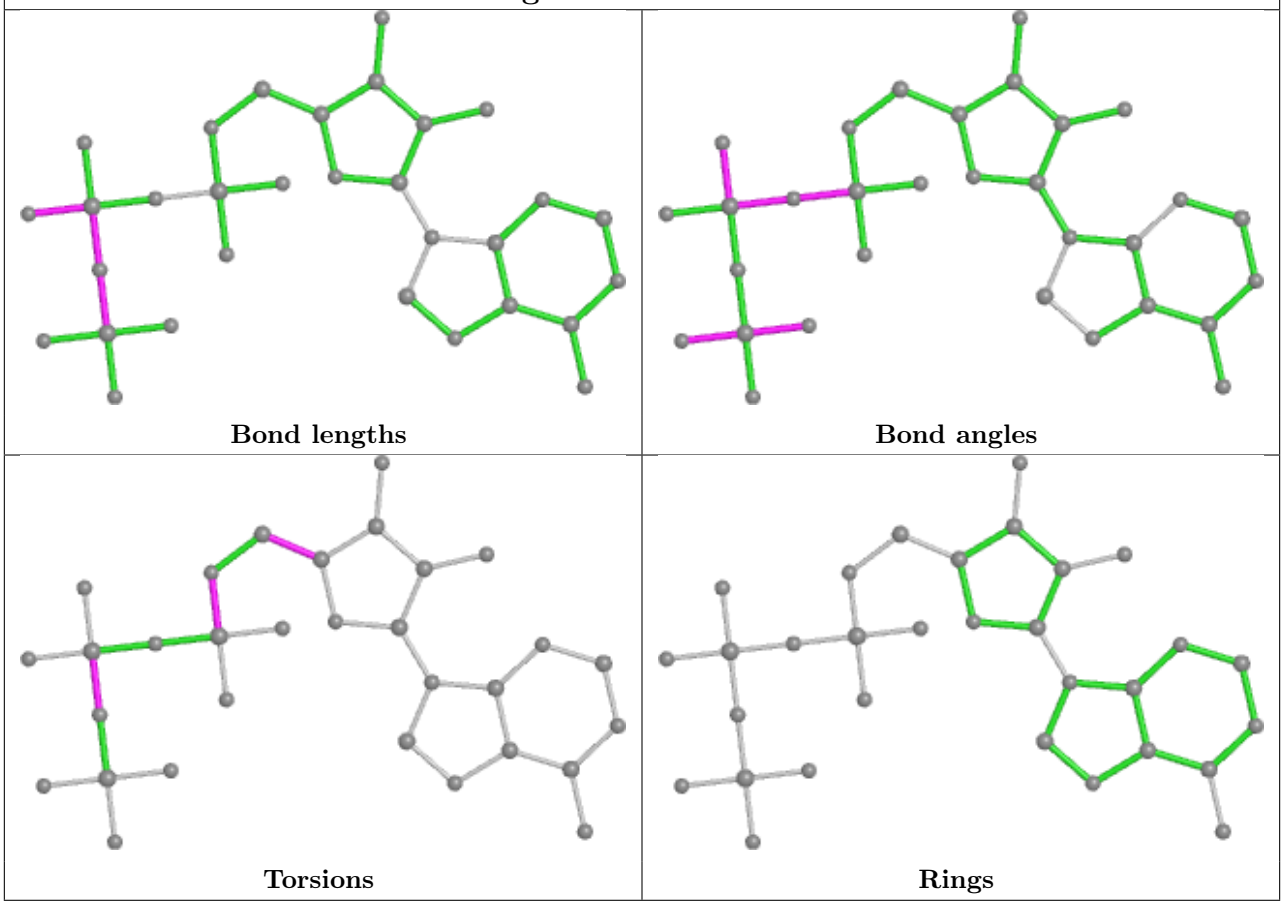
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ANP	1	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 ANP A 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	846/879 (96%)	-0.17	15 (1%) 68 48	27, 53, 89, 147	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	850	ASP	7.9
1	A	794	ASP	4.1
1	A	853	GLN	3.5
1	A	807	PRO	3.4
1	A	405	LYS	3.2
1	A	780	ARG	3.2
1	A	786	GLU	2.6
1	A	784	GLU	2.6
1	A	430	SER	2.5
1	A	864	GLU	2.5
1	A	73	MET	2.3
1	A	795	ILE	2.2
1	A	762	LYS	2.1
1	A	865	ILE	2.1
1	A	854	ILE	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

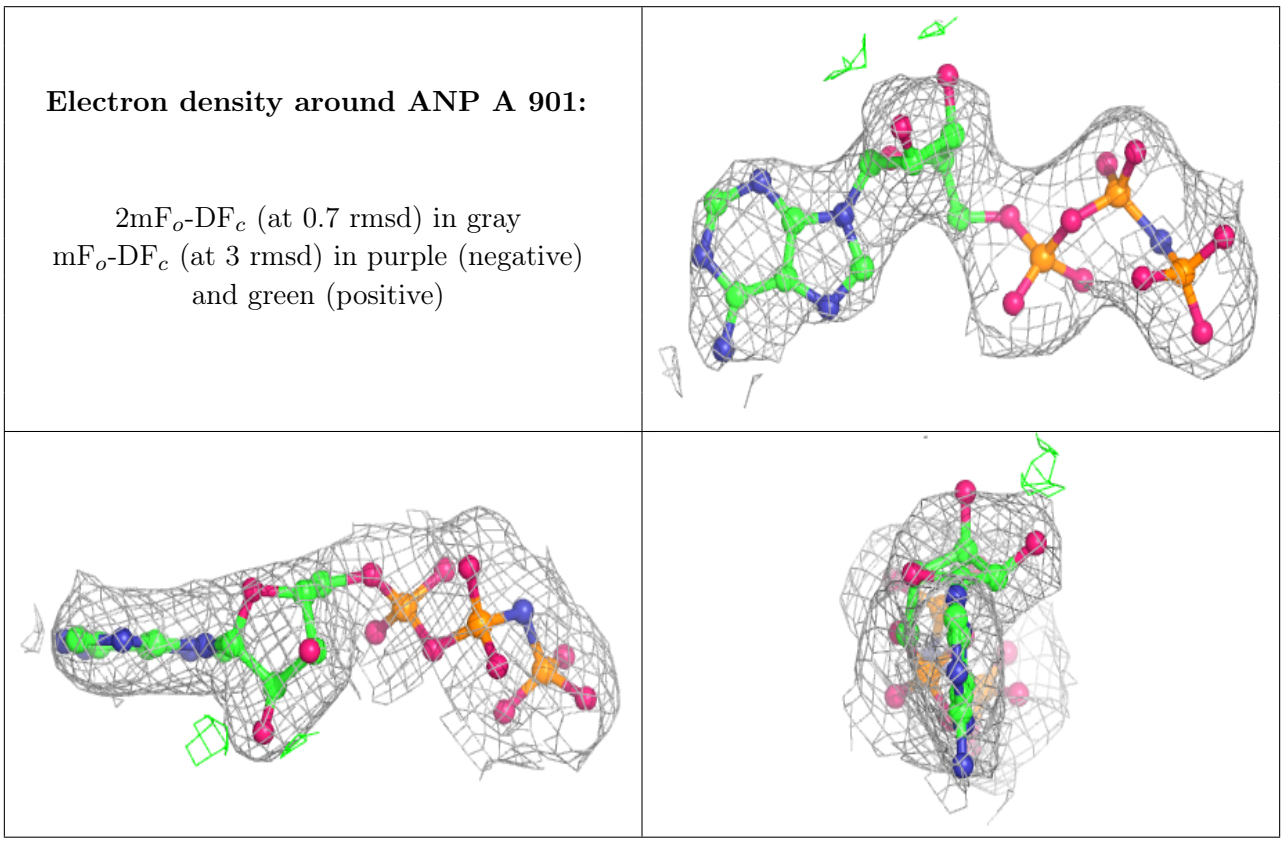
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	902	1/1	0.90	0.19	65,65,65,65	0
2	ANP	A	901	31/31	0.94	0.22	46,59,77,82	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 ANP A 901:

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.