Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:14 am BST

PDB ID	:	5CB2
Title	:	the structure of candida albicans Sey1p in complex with GMPPNP
Authors	:	Yan, L.; Sun, S.; Wang, W.; Shi, J.; Hu, X.; Wang, S.; Rao, Z.; Hu, J.; Lou, Z.
Deposited on	:	2015-06-30
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

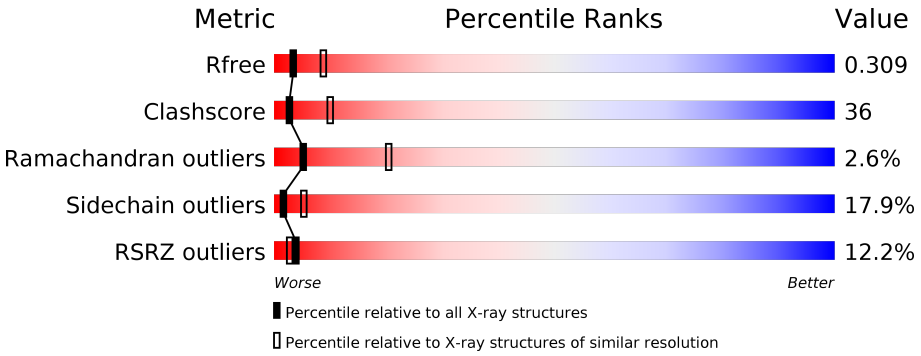
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	692	12% 40% 40% 13% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5357 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 Protein SEY1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	0	0
			5303	3390	877	1025	11			

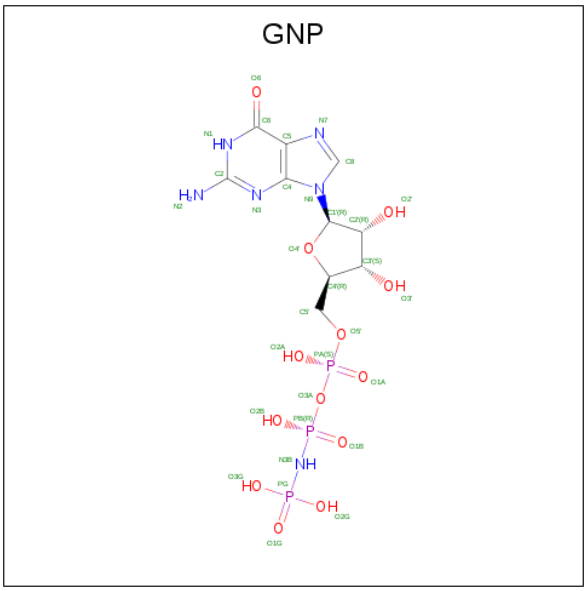
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	LEU	SER	see sequence details	UNP Q9C0L9
A	221	LEU	SER	see sequence details	UNP Q9C0L9
A	270	GLY	ASP	see sequence details	UNP Q9C0L9
A	337	THR	ALA	see sequence details	UNP Q9C0L9
A	479	VAL	ILE	see sequence details	UNP Q9C0L9
A	665	LEU	SER	see sequence details	UNP Q9C0L9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is water.

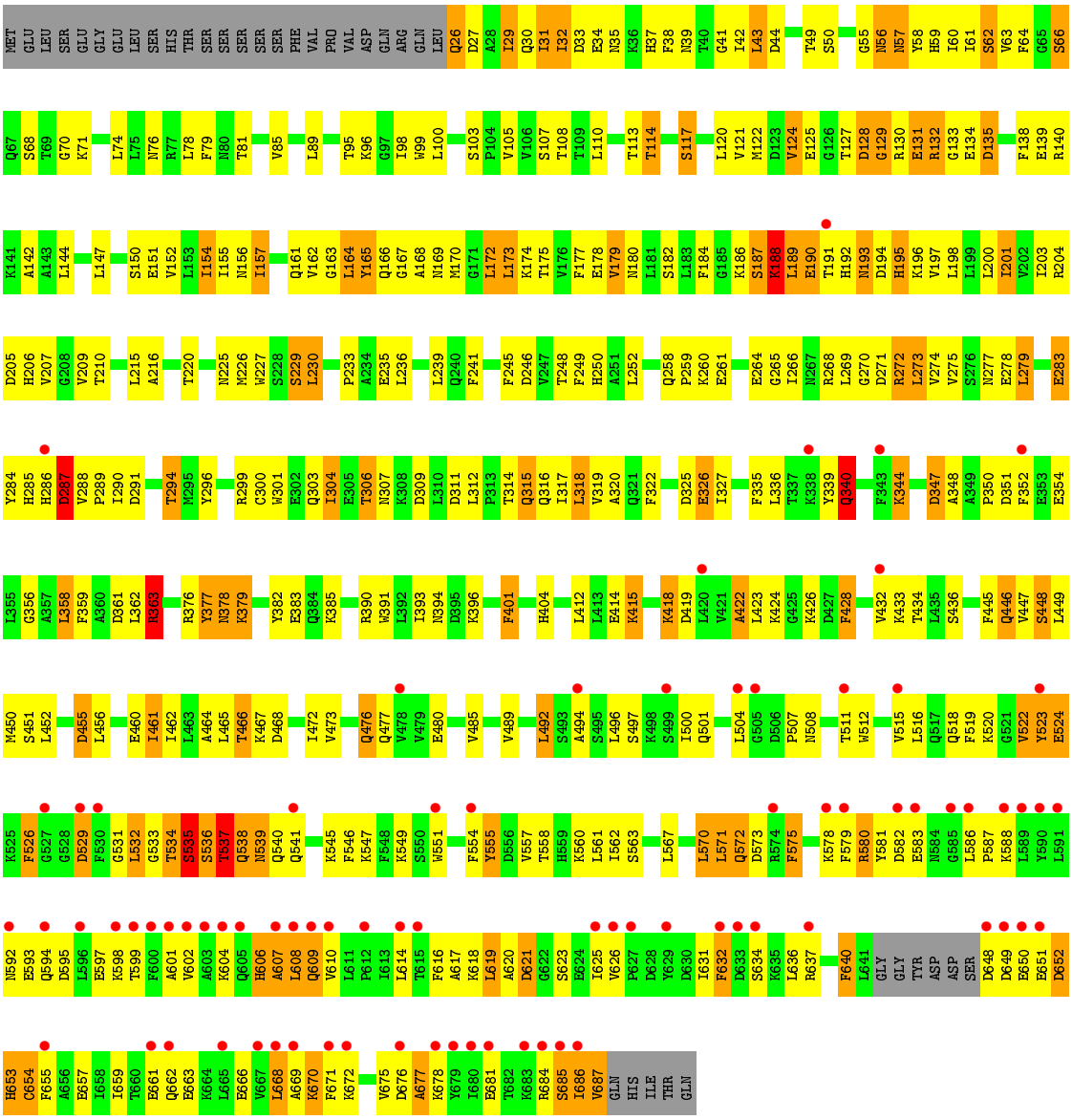
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		

3 Residue-property plots (i)

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

- Molecule 1: Protein SEY1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.57Å 120.93Å 190.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.90) 99.4 (48.87-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.260 , 0.298 0.276 , 0.309	Depositor DCC
R_{free} test set	1015 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 82.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5357	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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: GNP, MG

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	0.64	0/5404	1.01	43/7301 (0.6%)

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	1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	632	PHE	N-CA-CB	-11.43	90.03	110.60
1	A	607	ALA	CB-CA-C	9.72	124.69	110.10
1	A	58	TYR	N-CA-CB	-8.97	94.46	110.60
1	A	165	TYR	CB-CA-C	8.85	128.11	110.40
1	A	677	ALA	CB-CA-C	8.78	123.28	110.10
1	A	631	ILE	N-CA-C	8.65	134.34	111.00
1	A	320	ALA	CB-CA-C	-8.63	97.16	110.10
1	A	422	ALA	CB-CA-C	8.09	122.23	110.10
1	A	193	ASN	N-CA-CB	7.89	124.81	110.60
1	A	523	TYR	CB-CA-C	7.83	126.06	110.40
1	A	535	SER	N-CA-C	-7.65	90.34	111.00
1	A	524	GLU	N-CA-C	7.42	131.04	111.00
1	A	662	GLN	N-CA-CB	-7.25	97.54	110.60
1	A	166	GLN	N-CA-CB	-7.15	97.73	110.60
1	A	304	ILE	CB-CA-C	-7.11	97.38	111.60
1	A	526	PHE	CB-CA-C	7.02	124.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	GLN	N-CA-C	-6.98	92.15	111.00
1	A	522	VAL	CB-CA-C	-6.82	98.45	111.40
1	A	57	ASN	N-CA-C	6.81	129.40	111.00
1	A	279	LEU	CB-CA-C	-6.77	97.34	110.20
1	A	340	GLN	CB-CA-C	6.72	123.84	110.40
1	A	358	LEU	CB-CA-C	-6.56	97.73	110.20
1	A	56	ASN	N-CA-C	-6.41	93.71	111.00
1	A	306	THR	N-CA-C	6.34	128.13	111.00
1	A	609	GLN	N-CA-C	6.12	127.52	111.00
1	A	537	THR	CB-CA-C	6.05	127.95	111.60
1	A	494	ALA	N-CA-C	5.89	126.89	111.00
1	A	187	SER	N-CA-C	-5.83	95.25	111.00
1	A	179	VAL	CB-CA-C	-5.80	100.38	111.40
1	A	494	ALA	CB-CA-C	-5.75	101.47	110.10
1	A	188	LYS	N-CA-CB	5.63	120.73	110.60
1	A	608	LEU	N-CA-C	5.58	126.06	111.00
1	A	279	LEU	N-CA-C	5.56	126.01	111.00
1	A	291	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	492	LEU	CB-CA-C	-5.48	99.79	110.20
1	A	661	GLU	CB-CA-C	5.44	121.27	110.40
1	A	378	ASN	CB-CA-C	5.29	120.98	110.40
1	A	187	SER	CB-CA-C	5.28	120.14	110.10
1	A	363	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	287	ASP	N-CA-C	5.13	124.86	111.00
1	A	608	LEU	N-CA-CB	-5.13	100.14	110.40
1	A	678	LYS	N-CA-CB	-5.13	101.37	110.60
1	A	538	GLN	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	HIS	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	5303	0	5244	380	1
2	A	1	0	0	0	0
3	A	32	0	13	8	0
4	A	21	0	0	1	0
All	All	5357	0	5257	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 36.

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:619:LEU:CD1	1:A:621:ASP:OD1	1.64	1.44
1:A:194:ASP:OD2	1:A:196:LYS:N	1.61	1.33
1:A:192:HIS:HB2	1:A:193:ASN:C	1.51	1.29
1:A:193:ASN:ND2	1:A:287:ASP:HB2	1.59	1.17
1:A:619:LEU:HD12	1:A:621:ASP:OD1	1.29	1.10
1:A:677:ALA:O	1:A:681:GLU:HB3	1.47	1.10
1:A:619:LEU:HD13	1:A:621:ASP:OD1	1.52	1.07
1:A:194:ASP:OD2	1:A:195:HIS:C	1.92	1.07
1:A:534:THR:OG1	1:A:536:SER:N	1.87	1.06
1:A:535:SER:OG	1:A:538:GLN:HB2	1.57	1.04
1:A:188:LYS:HD3	1:A:189:LEU:H	1.16	1.02
1:A:130:ARG:HB2	1:A:131:GLU:OE1	1.58	1.02
1:A:63:VAL:O	1:A:124:VAL:CG1	2.09	1.00
1:A:193:ASN:ND2	1:A:287:ASP:CB	2.24	0.99
1:A:192:HIS:CB	1:A:193:ASN:C	2.31	0.99
1:A:677:ALA:O	1:A:681:GLU:CB	2.12	0.97
1:A:523:TYR:OH	1:A:551:TRP:NE1	1.86	0.95
1:A:127:THR:O	1:A:128:ASP:HB2	1.69	0.92
1:A:300:CYS:O	1:A:304:ILE:HG12	1.71	0.90
1:A:144:LEU:HD23	1:A:304:ILE:HG23	1.55	0.88
1:A:582:ASP:HB2	1:A:588:LYS:HA	1.52	0.88
1:A:192:HIS:HB2	1:A:194:ASP:N	1.90	0.85
1:A:68:SER:H	3:A:702:GNP:HNB3	1.25	0.84
1:A:188:LYS:N	1:A:190:GLU:OE1	2.11	0.84
1:A:193:ASN:HD21	1:A:287:ASP:HB2	1.40	0.83
1:A:358:LEU:HG	1:A:358:LEU:O	1.77	0.83
1:A:227:TRP:O	1:A:230:LEU:HD12	1.79	0.82
1:A:652:ASP:O	1:A:653:HIS:C	2.16	0.82
1:A:127:THR:O	1:A:128:ASP:CB	2.28	0.82
1:A:144:LEU:HD23	1:A:304:ILE:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:TYR:HA	1:A:587:PRO:HA	1.62	0.81
1:A:193:ASN:HD21	1:A:287:ASP:CB	1.90	0.81
1:A:537:THR:O	1:A:540:GLN:HB2	1.83	0.79
1:A:161:GLN:NE2	1:A:167:GLY:O	2.14	0.79
1:A:325:ASP:OD1	1:A:385:LYS:HD2	1.82	0.79
1:A:189:LEU:HD22	1:A:189:LEU:O	1.83	0.79
1:A:144:LEU:CD2	1:A:304:ILE:HD12	2.13	0.78
1:A:235:GLU:HG2	1:A:236:LEU:HG	1.62	0.78
1:A:130:ARG:CB	1:A:131:GLU:OE1	2.30	0.78
1:A:155:ILE:O	1:A:201:ILE:HD12	1.84	0.78
1:A:619:LEU:CD1	1:A:621:ASP:CG	2.51	0.77
1:A:340:GLN:O	1:A:344:LYS:HB2	1.82	0.77
1:A:588:LYS:HE2	1:A:599:THR:HG21	1.65	0.77
1:A:193:ASN:HD21	1:A:287:ASP:CG	1.88	0.76
1:A:193:ASN:ND2	1:A:287:ASP:OD2	2.18	0.76
1:A:507:PRO:HB3	1:A:610:VAL:HG23	1.68	0.76
1:A:154:ILE:HA	1:A:200:LEU:O	1.85	0.76
1:A:619:LEU:HD11	1:A:621:ASP:HB2	1.67	0.76
1:A:187:SER:HA	1:A:190:GLU:OE1	1.85	0.75
1:A:619:LEU:HD12	1:A:621:ASP:CG	2.07	0.75
1:A:492:LEU:O	1:A:496:LEU:CB	2.35	0.74
1:A:335:PHE:CZ	1:A:393:ILE:HG23	2.23	0.73
1:A:522:VAL:CG1	1:A:522:VAL:O	2.37	0.72
1:A:260:LYS:O	1:A:264:GLU:HG3	1.88	0.72
1:A:63:VAL:O	1:A:124:VAL:HG12	1.90	0.72
1:A:193:ASN:O	1:A:286:HIS:HD2	1.73	0.71
1:A:516:LEU:HA	1:A:519:PHE:HB3	1.71	0.71
1:A:534:THR:HG1	1:A:536:SER:H	1.35	0.71
1:A:68:SER:N	3:A:702:GNP:HNB3	1.88	0.70
1:A:582:ASP:HB2	1:A:588:LYS:CA	2.21	0.70
1:A:70:GLY:HA2	3:A:702:GNP:O1A	1.91	0.70
1:A:522:VAL:O	1:A:522:VAL:HG12	1.90	0.69
1:A:535:SER:HG	1:A:538:GLN:HB2	1.55	0.69
1:A:107:SER:O	1:A:270:GLY:HA3	1.92	0.69
1:A:205:ASP:OD1	3:A:702:GNP:N1	2.19	0.69
1:A:602:VAL:O	1:A:606:HIS:HB2	1.92	0.69
1:A:55:GLY:O	1:A:289:PRO:HA	1.92	0.69
1:A:531:GLY:O	1:A:532:LEU:O	2.10	0.69
1:A:130:ARG:O	1:A:131:GLU:C	2.29	0.68
1:A:581:TYR:CZ	1:A:587:PRO:HG3	2.28	0.68
1:A:582:ASP:CB	1:A:588:LYS:HA	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:O	1:A:170:MET:HB2	1.93	0.68
1:A:57:ASN:O	1:A:57:ASN:CG	2.28	0.68
1:A:572:GLN:HA	1:A:575:PHE:HB3	1.75	0.68
1:A:31:ILE:HG23	1:A:42:ILE:HD13	1.75	0.67
1:A:192:HIS:CB	1:A:193:ASN:O	2.43	0.67
1:A:31:ILE:HD11	1:A:98:ILE:HG22	1.76	0.67
1:A:492:LEU:O	1:A:496:LEU:HB3	1.94	0.67
1:A:192:HIS:HB2	1:A:193:ASN:O	1.93	0.67
1:A:227:TRP:O	1:A:230:LEU:CD1	2.43	0.66
1:A:38:PHE:HB2	1:A:301:TRP:CD1	2.31	0.66
1:A:205:ASP:CG	3:A:702:GNP:HN1	1.98	0.66
1:A:492:LEU:O	1:A:496:LEU:HB2	1.94	0.66
1:A:63:VAL:HG23	1:A:154:ILE:CG1	2.25	0.66
1:A:201:ILE:HG12	1:A:249:PHE:HE1	1.61	0.66
1:A:512:TRP:CD1	1:A:618:LYS:O	2.49	0.66
1:A:38:PHE:HB2	1:A:301:TRP:HD1	1.61	0.66
1:A:188:LYS:HD3	1:A:189:LEU:N	2.01	0.65
1:A:619:LEU:HD11	1:A:621:ASP:CB	2.25	0.65
1:A:131:GLU:OE1	1:A:131:GLU:N	2.30	0.65
1:A:428:PHE:CB	1:A:532:LEU:HA	2.27	0.65
1:A:583:GLU:OE1	1:A:583:GLU:HA	1.95	0.65
1:A:192:HIS:CB	1:A:193:ASN:CA	2.74	0.65
1:A:194:ASP:OD2	1:A:195:HIS:N	2.30	0.65
1:A:452:LEU:O	1:A:455:ASP:HB2	1.95	0.65
1:A:523:TYR:OH	1:A:551:TRP:CD1	2.41	0.64
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.80	0.64
1:A:428:PHE:HE2	1:A:477:GLN:HG3	1.62	0.64
1:A:534:THR:OG1	1:A:535:SER:N	2.30	0.64
1:A:684:ARG:O	1:A:687:VAL:HB	1.97	0.64
1:A:557:VAL:O	1:A:561:LEU:HB2	1.98	0.64
1:A:29:ILE:H	1:A:29:ILE:HD12	1.63	0.63
1:A:100:LEU:HD12	1:A:122:MET:HG3	1.81	0.63
1:A:177:PHE:O	1:A:180:ASN:HB3	1.99	0.63
1:A:63:VAL:O	1:A:124:VAL:HG11	1.99	0.63
1:A:130:ARG:O	1:A:132:ARG:C	2.37	0.63
1:A:485:VAL:HG22	1:A:526:PHE:CZ	2.33	0.63
1:A:139:GLU:HG3	1:A:172:LEU:CD2	2.29	0.62
1:A:377:TYR:HD1	1:A:377:TYR:H	1.46	0.62
1:A:57:ASN:O	1:A:117:SER:CB	2.48	0.62
1:A:563:SER:O	1:A:567:LEU:HB2	2.00	0.62
1:A:26:GLN:CG	1:A:26:GLN:O	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ALA:O	1:A:424:LYS:HE3	1.98	0.62
1:A:128:ASP:OD1	1:A:129:GLY:N	2.29	0.61
1:A:78:LEU:HD22	1:A:269:LEU:HD23	1.80	0.61
1:A:306:THR:O	1:A:306:THR:OG1	2.19	0.61
1:A:464:ALA:HA	1:A:467:LYS:HG2	1.81	0.61
1:A:489:VAL:HG12	1:A:489:VAL:O	2.00	0.61
1:A:108:THR:HB	1:A:271:ASP:OD1	2.00	0.61
1:A:290:ILE:O	1:A:294:THR:HG23	1.99	0.61
1:A:547:LYS:O	1:A:551:TRP:HD1	1.82	0.61
1:A:619:LEU:CD1	1:A:621:ASP:CB	2.80	0.60
1:A:619:LEU:HD12	1:A:621:ASP:N	2.16	0.60
1:A:193:ASN:HD22	1:A:287:ASP:CB	2.13	0.60
1:A:376:ARG:HD2	1:A:377:TYR:HE1	1.67	0.59
1:A:390:ARG:HG2	1:A:391:TRP:CD1	2.36	0.59
1:A:134:GLU:O	1:A:314:THR:HG21	2.02	0.59
1:A:377:TYR:CD1	1:A:377:TYR:N	2.70	0.59
1:A:428:PHE:HB3	1:A:532:LEU:HA	1.85	0.59
1:A:130:ARG:O	1:A:132:ARG:N	2.36	0.58
1:A:193:ASN:ND2	1:A:287:ASP:CG	2.53	0.58
1:A:230:LEU:HD12	1:A:230:LEU:H	1.69	0.58
1:A:311:ASP:O	1:A:312:LEU:HD23	2.02	0.58
1:A:352:PHE:CE2	1:A:446:GLN:HG3	2.39	0.58
1:A:61:ILE:HD12	1:A:152:VAL:O	2.04	0.58
1:A:63:VAL:HG23	1:A:154:ILE:HG13	1.84	0.58
1:A:139:GLU:HG3	1:A:172:LEU:HD21	1.85	0.58
1:A:534:THR:OG1	1:A:536:SER:CA	2.52	0.58
1:A:29:ILE:HD12	1:A:100:LEU:O	2.04	0.57
1:A:61:ILE:CD1	1:A:152:VAL:HB	2.34	0.57
1:A:571:LEU:HB2	1:A:572:GLN:OE1	2.04	0.57
1:A:432:VAL:O	1:A:436:SER:HB2	2.05	0.57
1:A:512:TRP:CG	1:A:618:LYS:O	2.58	0.57
1:A:174:LYS:HG3	1:A:229:SER:OG	2.04	0.57
1:A:283:GLU:OE1	1:A:283:GLU:N	2.36	0.57
1:A:273:LEU:HB3	1:A:279:LEU:CD2	2.34	0.57
1:A:187:SER:CA	1:A:190:GLU:OE1	2.52	0.57
1:A:113:THR:HG22	1:A:114:THR:O	2.04	0.57
1:A:379:LYS:O	1:A:383:GLU:N	2.30	0.56
1:A:582:ASP:O	1:A:586:LEU:HB2	2.05	0.56
1:A:161:GLN:O	1:A:164:LEU:HB2	2.06	0.56
1:A:226:MET:O	1:A:226:MET:HG2	2.04	0.56
1:A:273:LEU:HB3	1:A:279:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:HA	1:A:164:LEU:HD22	1.88	0.56
1:A:501:GLN:HA	1:A:504:LEU:HB2	1.89	0.55
1:A:428:PHE:HB2	1:A:532:LEU:HA	1.89	0.55
1:A:79:PHE:HB3	1:A:103:SER:HB2	1.87	0.55
1:A:38:PHE:CD1	1:A:39:ASN:N	2.74	0.55
1:A:555:TYR:CD1	1:A:555:TYR:C	2.80	0.55
1:A:178:GLU:N	1:A:230:LEU:HD23	2.21	0.55
1:A:501:GLN:O	1:A:504:LEU:N	2.41	0.54
1:A:536:SER:HA	1:A:539:ASN:HB3	1.90	0.54
1:A:99:TRP:O	1:A:122:MET:HA	2.08	0.54
1:A:241:PHE:O	1:A:245:PHE:HB2	2.08	0.54
1:A:272:ARG:HD3	1:A:278:GLU:OE2	2.07	0.54
1:A:554:PHE:O	1:A:558:THR:HG23	2.08	0.54
1:A:132:ARG:CG	1:A:132:ARG:O	2.56	0.53
1:A:193:ASN:O	1:A:286:HIS:CD2	2.60	0.53
1:A:194:ASP:OD2	1:A:195:HIS:CA	2.56	0.53
1:A:201:ILE:HG12	1:A:249:PHE:CE1	2.42	0.53
1:A:686:ILE:O	1:A:687:VAL:O	2.27	0.53
1:A:216:ALA:O	1:A:220:THR:HG23	2.09	0.53
1:A:154:ILE:HG22	1:A:200:LEU:HD23	1.91	0.53
1:A:144:LEU:HD23	1:A:304:ILE:CG2	2.32	0.53
1:A:315:GLN:O	1:A:319:VAL:HG23	2.10	0.52
1:A:515:VAL:HG12	1:A:516:LEU:HD12	1.90	0.52
1:A:571:LEU:HD23	1:A:607:ALA:HB1	1.90	0.52
1:A:130:ARG:O	1:A:133:GLY:N	2.43	0.52
1:A:634:SER:HA	1:A:637:ARG:HB2	1.90	0.52
1:A:265:GLY:HA2	1:A:268:ARG:CZ	2.40	0.52
1:A:192:HIS:HB3	1:A:193:ASN:HB3	1.91	0.52
1:A:539:ASN:HD22	1:A:539:ASN:C	2.14	0.52
1:A:201:ILE:CG2	1:A:249:PHE:CE1	2.93	0.51
1:A:78:LEU:CD2	1:A:269:LEU:HD23	2.40	0.51
1:A:138:PHE:O	1:A:138:PHE:CD1	2.64	0.51
1:A:322:PHE:CD1	1:A:322:PHE:C	2.83	0.51
1:A:520:LYS:HA	1:A:523:TYR:HB3	1.92	0.51
1:A:485:VAL:HG22	1:A:526:PHE:HZ	1.74	0.51
1:A:66:SER:HA	1:A:127:THR:O	2.10	0.51
1:A:201:ILE:HG23	1:A:249:PHE:CE1	2.46	0.51
1:A:570:LEU:HA	1:A:573:ASP:OD2	2.10	0.51
1:A:140:ARG:HA	1:A:172:LEU:HD11	1.93	0.51
1:A:358:LEU:CG	1:A:358:LEU:O	2.51	0.51
1:A:31:ILE:HD11	1:A:98:ILE:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:HD2	1:A:377:TYR:CE1	2.45	0.51
1:A:529:ASP:OD1	1:A:529:ASP:N	2.44	0.51
1:A:128:ASP:O	1:A:129:GLY:O	2.29	0.51
1:A:299:ARG:O	1:A:303:GLN:HG3	2.11	0.51
1:A:512:TRP:HB2	1:A:619:LEU:O	2.11	0.51
1:A:132:ARG:O	1:A:132:ARG:HG3	2.10	0.51
1:A:178:GLU:HG3	1:A:230:LEU:HB2	1.92	0.51
1:A:347:ASP:C	1:A:347:ASP:OD1	2.49	0.51
1:A:651:GLU:O	1:A:652:ASP:CB	2.58	0.51
1:A:140:ARG:HG2	1:A:172:LEU:HD13	1.93	0.50
1:A:56:ASN:ND2	1:A:287:ASP:OD1	2.37	0.50
1:A:446:GLN:OE1	1:A:446:GLN:HA	2.12	0.50
1:A:31:ILE:CG2	1:A:42:ILE:HD13	2.42	0.50
1:A:325:ASP:OD1	1:A:385:LYS:CD	2.57	0.50
1:A:659:ILE:HG13	1:A:663:GLU:HB2	1.92	0.50
1:A:401:PHE:CD1	1:A:401:PHE:C	2.84	0.50
1:A:508:ASN:H	1:A:511:THR:HG23	1.77	0.50
1:A:173:LEU:O	1:A:174:LYS:C	2.50	0.50
1:A:326:GLU:HG2	1:A:327:ILE:N	2.27	0.50
1:A:186:LYS:O	1:A:188:LYS:N	2.44	0.49
1:A:26:GLN:O	1:A:26:GLN:HG2	2.13	0.49
1:A:476:GLN:HE21	1:A:476:GLN:HA	1.78	0.49
1:A:533:GLY:O	1:A:534:THR:C	2.50	0.49
1:A:652:ASP:O	1:A:653:HIS:O	2.30	0.49
1:A:127:THR:O	1:A:127:THR:OG1	2.29	0.49
1:A:592:ASN:HB3	1:A:594:GLN:HB2	1.94	0.49
1:A:507:PRO:HB3	1:A:610:VAL:CG2	2.40	0.49
1:A:60:ILE:HD13	1:A:120:LEU:HB2	1.94	0.49
1:A:62:SER:OG	1:A:150:SER:OG	2.29	0.49
1:A:227:TRP:CG	1:A:241:PHE:HB2	2.47	0.49
1:A:250:HIS:NE2	1:A:269:LEU:HB2	2.27	0.49
1:A:352:PHE:HE2	1:A:446:GLN:HG3	1.77	0.49
1:A:29:ILE:N	1:A:29:ILE:HD12	2.28	0.48
1:A:592:ASN:C	1:A:594:GLN:H	2.17	0.48
1:A:351:ASP:HB3	1:A:354:GLU:CD	2.33	0.48
1:A:537:THR:HA	1:A:540:GLN:OE1	2.13	0.48
1:A:57:ASN:O	1:A:117:SER:HA	2.14	0.48
1:A:686:ILE:HG23	1:A:686:ILE:O	2.12	0.48
1:A:378:ASN:O	1:A:382:TYR:HB3	2.14	0.48
1:A:651:GLU:O	1:A:652:ASP:HB3	2.14	0.48
1:A:188:LYS:C	1:A:190:GLU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:HIS:HE1	1:A:210:THR:O	1.96	0.48
1:A:315:GLN:O	1:A:316:GLN:C	2.52	0.48
1:A:545:LYS:CG	1:A:640:PHE:HD2	2.27	0.48
1:A:671:PHE:HD1	1:A:672:LYS:HG3	1.78	0.48
1:A:64:PHE:CE1	1:A:127:THR:HG21	2.49	0.47
1:A:128:ASP:CG	1:A:129:GLY:H	2.13	0.47
1:A:376:ARG:HB2	1:A:377:TYR:CD1	2.49	0.47
1:A:165:TYR:O	1:A:170:MET:N	2.46	0.47
1:A:250:HIS:CD2	1:A:269:LEU:HB2	2.49	0.47
1:A:188:LYS:O	1:A:190:GLU:HG3	2.14	0.47
1:A:677:ALA:O	1:A:681:GLU:HB2	2.12	0.47
1:A:685:SER:C	1:A:687:VAL:H	2.18	0.47
1:A:30:GLN:HB3	1:A:99:TRP:CE2	2.48	0.47
1:A:56:ASN:OD1	1:A:285:HIS:HE1	1.98	0.47
1:A:168:ALA:O	1:A:169:ASN:HB2	2.13	0.47
1:A:139:GLU:HG3	1:A:172:LEU:HD22	1.95	0.47
1:A:545:LYS:O	1:A:549:LYS:HG3	2.14	0.47
1:A:189:LEU:CD2	1:A:189:LEU:O	2.61	0.47
1:A:348:ALA:O	1:A:350:PRO:HD3	2.14	0.46
1:A:451:SER:HB2	1:A:456:LEU:O	2.15	0.46
1:A:76:ASN:HA	1:A:81:THR:OG1	2.15	0.46
1:A:43:LEU:HG	1:A:294:THR:HG21	1.97	0.46
1:A:533:GLY:C	1:A:534:THR:O	2.50	0.46
1:A:124:VAL:HG22	1:A:125:GLU:O	2.15	0.46
1:A:445:PHE:O	1:A:449:LEU:HG	2.15	0.46
1:A:32:ILE:HG23	1:A:98:ILE:HB	1.97	0.46
1:A:61:ILE:HD12	1:A:152:VAL:HB	1.98	0.46
1:A:531:GLY:C	1:A:532:LEU:O	2.54	0.46
1:A:545:LYS:HG2	1:A:640:PHE:HB3	1.96	0.46
1:A:130:ARG:HB3	1:A:131:GLU:H	1.48	0.46
1:A:261:GLU:N	1:A:261:GLU:OE1	2.45	0.46
1:A:533:GLY:O	1:A:534:THR:O	2.34	0.46
1:A:140:ARG:HA	1:A:172:LEU:CD1	2.46	0.46
1:A:157:ILE:CG1	1:A:201:ILE:HD11	2.46	0.45
1:A:524:GLU:O	1:A:524:GLU:OE1	2.33	0.45
1:A:351:ASP:HB3	1:A:354:GLU:HB2	1.98	0.45
1:A:512:TRP:HA	1:A:515:VAL:HB	1.98	0.45
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.41	0.45
1:A:419:ASP:O	1:A:423:LEU:HD23	2.16	0.45
1:A:601:ALA:HA	1:A:604:LYS:HG3	1.98	0.45
1:A:619:LEU:HD12	1:A:621:ASP:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD12	1:A:147:LEU:O	2.16	0.45
1:A:201:ILE:HG23	1:A:249:PHE:CD1	2.52	0.45
1:A:201:ILE:O	1:A:249:PHE:HA	2.17	0.45
1:A:95:THR:HB	1:A:125:GLU:HA	1.99	0.45
1:A:135:ASP:OD1	1:A:135:ASP:O	2.34	0.45
1:A:250:HIS:CG	1:A:269:LEU:HD13	2.51	0.45
1:A:33:ASP:OD1	1:A:33:ASP:C	2.54	0.45
1:A:654:CYS:HB3	1:A:657:GLU:HB2	1.99	0.45
1:A:467:LYS:HG3	1:A:468:ASP:N	2.32	0.44
1:A:685:SER:C	1:A:687:VAL:N	2.70	0.44
1:A:414:GLU:O	1:A:415:LYS:C	2.56	0.44
1:A:519:PHE:O	1:A:523:TYR:HB2	2.17	0.44
1:A:594:GLN:O	1:A:598:LYS:HB2	2.16	0.44
1:A:68:SER:CA	3:A:702:GNP:HNB3	2.29	0.44
1:A:582:ASP:HB2	1:A:588:LYS:HG3	2.00	0.44
1:A:350:PRO:HB3	1:A:404:HIS:HD2	1.82	0.44
1:A:625:ILE:HG22	1:A:655:PHE:HE2	1.81	0.44
1:A:246:ASP:OD2	1:A:284:TYR:OH	2.21	0.44
1:A:520:LYS:NZ	1:A:551:TRP:CZ2	2.84	0.44
1:A:520:LYS:HZ1	1:A:551:TRP:HZ2	1.63	0.44
1:A:61:ILE:HD13	1:A:152:VAL:HB	1.98	0.44
1:A:179:VAL:CG1	1:A:179:VAL:O	2.63	0.44
1:A:538:GLN:HA	1:A:541:GLN:HB2	2.00	0.44
1:A:575:PHE:HE2	1:A:675:VAL:HG13	1.82	0.44
1:A:33:ASP:OD2	1:A:37:HIS:HB3	2.18	0.43
1:A:593:GLU:O	1:A:597:GLU:HB2	2.17	0.43
1:A:63:VAL:O	1:A:124:VAL:HG13	2.09	0.43
1:A:317:ILE:O	1:A:318:LEU:C	2.56	0.43
1:A:363:ARG:HB3	1:A:363:ARG:HH11	1.82	0.43
1:A:49:THR:OG1	1:A:50:SER:N	2.52	0.43
1:A:98:ILE:HD11	1:A:142:ALA:HB1	2.01	0.43
1:A:162:VAL:HG12	1:A:163:GLY:N	2.33	0.43
1:A:258:GLN:N	1:A:259:PRO:HD3	2.34	0.43
1:A:34:GLU:HG3	1:A:96:LYS:HB3	2.00	0.43
1:A:547:LYS:O	1:A:551:TRP:CD1	2.68	0.43
1:A:62:SER:HB3	1:A:122:MET:HB2	2.01	0.43
1:A:233:PRO:HG2	1:A:236:LEU:HD12	2.02	0.42
1:A:152:VAL:HG22	1:A:198:LEU:HB3	2.01	0.42
1:A:57:ASN:O	1:A:117:SER:CA	2.68	0.42
1:A:356:GLY:O	1:A:359:PHE:HB2	2.19	0.42
1:A:473:VAL:O	1:A:477:GLN:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:GLN:O	1:A:476:GLN:HG3	2.18	0.42
1:A:57:ASN:O	1:A:117:SER:HB3	2.20	0.42
1:A:578:LYS:C	1:A:580:ARG:H	2.23	0.42
1:A:669:ALA:C	1:A:670:LYS:HG2	2.38	0.42
1:A:296:TYR:O	1:A:300:CYS:SG	2.53	0.42
1:A:578:LYS:C	1:A:580:ARG:N	2.73	0.42
1:A:608:LEU:HD21	1:A:668:LEU:HD11	2.00	0.42
1:A:63:VAL:HG22	1:A:71:LYS:HD2	2.01	0.42
1:A:192:HIS:HB3	1:A:193:ASN:O	2.18	0.42
1:A:497:SER:HA	1:A:500:ILE:HD12	2.01	0.42
1:A:582:ASP:OD1	1:A:583:GLU:N	2.52	0.42
1:A:154:ILE:CG2	1:A:200:LEU:HD23	2.50	0.42
1:A:274:VAL:HG12	1:A:275:VAL:N	2.34	0.42
1:A:418:LYS:HE3	1:A:422:ALA:HB2	2.00	0.42
1:A:447:VAL:O	1:A:450:MET:HB3	2.19	0.42
1:A:396:LYS:HA	1:A:396:LYS:HD2	1.77	0.42
1:A:545:LYS:HG3	1:A:640:PHE:HD2	1.85	0.42
1:A:187:SER:C	1:A:190:GLU:OE1	2.58	0.41
1:A:192:HIS:HB3	1:A:193:ASN:CB	2.50	0.41
1:A:340:GLN:O	1:A:344:LYS:CB	2.62	0.41
1:A:567:LEU:HA	1:A:567:LEU:HD12	1.94	0.41
1:A:575:PHE:CD1	1:A:575:PHE:C	2.92	0.41
1:A:580:ARG:O	1:A:581:TYR:CD2	2.73	0.41
1:A:582:ASP:O	1:A:586:LEU:CB	2.68	0.41
1:A:61:ILE:HG23	1:A:121:VAL:HA	2.03	0.41
1:A:108:THR:HG22	1:A:270:GLY:C	2.41	0.41
1:A:138:PHE:C	1:A:138:PHE:CD1	2.93	0.41
1:A:157:ILE:HG13	1:A:157:ILE:H	1.61	0.41
1:A:465:LEU:O	1:A:466:THR:C	2.59	0.41
1:A:204:ARG:NH2	3:A:702:GNP:N7	2.68	0.41
1:A:451:SER:O	1:A:452:LEU:C	2.58	0.41
1:A:539:ASN:ND2	1:A:539:ASN:C	2.73	0.41
1:A:140:ARG:HD3	1:A:175:THR:HG21	2.02	0.41
1:A:192:HIS:CD2	1:A:194:ASP:HA	2.55	0.41
1:A:546:PHE:C	1:A:546:PHE:CD1	2.94	0.41
1:A:59:HIS:HA	1:A:151:GLU:OE1	2.21	0.41
1:A:561:LEU:HB3	1:A:562:ILE:HD12	2.02	0.41
1:A:156:ASN:HD21	1:A:204:ARG:HH11	1.68	0.41
1:A:225:ASN:O	1:A:226:MET:C	2.58	0.41
1:A:423:LEU:HD12	1:A:426:LYS:HD2	2.03	0.41
1:A:592:ASN:C	1:A:594:GLN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:CD1	1:A:203:ILE:HG12	2.51	0.41
1:A:192:HIS:HD2	1:A:194:ASP:HA	1.86	0.41
1:A:204:ARG:HA	1:A:204:ARG:HD2	1.89	0.41
1:A:144:LEU:CD2	1:A:304:ILE:HG23	2.38	0.41
1:A:461:ILE:HG22	1:A:462:ILE:N	2.36	0.41
1:A:501:GLN:O	1:A:504:LEU:HB2	2.21	0.41
1:A:578:LYS:O	1:A:580:ARG:N	2.54	0.41
1:A:207:VAL:HG23	1:A:209:VAL:H	1.86	0.40
1:A:38:PHE:HD1	1:A:39:ASN:N	2.18	0.40
1:A:68:SER:HA	3:A:702:GNP:HNB3	1.86	0.40
1:A:95:THR:O	1:A:125:GLU:HB2	2.20	0.40
1:A:307:ASN:O	1:A:311:ASP:HB2	2.22	0.40
1:A:526:PHE:HA	4:A:804:HOH:O	2.21	0.40
1:A:535:SER:O	1:A:535:SER:OG	2.30	0.40
1:A:472:ILE:O	1:A:473:VAL:C	2.58	0.40
1:A:428:PHE:HB2	1:A:532:LEU:HD23	2.04	0.40
1:A:194:ASP:OD2	1:A:194:ASP:C	2.59	0.40
1:A:203:ILE:HD13	1:A:215:LEU:HD13	2.03	0.40
1:A:391:TRP:HA	1:A:394:ASN:HB2	2.04	0.40
1:A:352:PHE:CD2	1:A:446:GLN:HG3	2.57	0.40
1:A:572:GLN:CD	1:A:572:GLN:N	2.75	0.40
1:A:666:GLU:O	1:A:670:LYS:HG3	2.21	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:580:ARG:NH2	1:A:587:PRO:CG[6_555]	2.06	0.14

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	652/692 (94%)	535 (82%)	100 (15%)	17 (3%)	5 20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ASP
1	A	129	GLY
1	A	131	GLU
1	A	315	GLN
1	A	532	LEU
1	A	620	ALA
1	A	652	ASP
1	A	650	GLU
1	A	191	THR
1	A	448	SER
1	A	579	PHE
1	A	617	ALA
1	A	536	SER
1	A	653	HIS
1	A	309	ASP
1	A	336	LEU
1	A	41	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	588/621 (95%)	483 (82%)	105 (18%)	2 5

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	ASP
1	A	29	ILE
1	A	31	ILE

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Mol	Chain	Res	Type
1	A	32	ILE
1	A	35	ASN
1	A	43	LEU
1	A	44	ASP
1	A	62	SER
1	A	66	SER
1	A	74	LEU
1	A	85	VAL
1	A	89	LEU
1	A	105	VAL
1	A	110	LEU
1	A	114	THR
1	A	117	SER
1	A	124	VAL
1	A	132	ARG
1	A	135	ASP
1	A	154	ILE
1	A	157	ILE
1	A	164	LEU
1	A	172	LEU
1	A	173	LEU
1	A	182	SER
1	A	184	PHE
1	A	188	LYS
1	A	189	LEU
1	A	190	GLU
1	A	197	VAL
1	A	201	ILE
1	A	229	SER
1	A	230	LEU
1	A	239	LEU
1	A	248	THR
1	A	252	LEU
1	A	266	ILE
1	A	272	ARG
1	A	273	LEU
1	A	277	ASN
1	A	283	GLU
1	A	287	ASP
1	A	288	VAL
1	A	294	THR
1	A	318	LEU

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Mol	Chain	Res	Type
1	A	326	GLU
1	A	339	TYR
1	A	340	GLN
1	A	344	LYS
1	A	347	ASP
1	A	361	ASP
1	A	362	LEU
1	A	363	ARG
1	A	377	TYR
1	A	379	LYS
1	A	401	PHE
1	A	412	LEU
1	A	415	LYS
1	A	418	LYS
1	A	428	PHE
1	A	433	LYS
1	A	434	THR
1	A	446	GLN
1	A	448	SER
1	A	455	ASP
1	A	460	GLU
1	A	461	ILE
1	A	466	THR
1	A	476	GLN
1	A	480	GLU
1	A	518	GLN
1	A	529	ASP
1	A	534	THR
1	A	535	SER
1	A	537	THR
1	A	539	ASN
1	A	555	TYR
1	A	560	LYS
1	A	570	LEU
1	A	571	LEU
1	A	572	GLN
1	A	575	PHE
1	A	580	ARG
1	A	595	ASP
1	A	606	HIS
1	A	609	GLN
1	A	614	LEU

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Mol	Chain	Res	Type
1	A	616	PHE
1	A	619	LEU
1	A	621	ASP
1	A	623	SER
1	A	626	VAL
1	A	632	PHE
1	A	636	LEU
1	A	640	PHE
1	A	648	ASP
1	A	649	ASP
1	A	654	CYS
1	A	668	LEU
1	A	670	LYS
1	A	676	ASP
1	A	685	SER
1	A	686	ILE
1	A	687	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	156	ASN
1	A	166	GLN
1	A	192	HIS
1	A	193	ASN
1	A	206	HIS
1	A	238	HIS
1	A	285	HIS
1	A	286	HIS
1	A	315	GLN
1	A	321	GLN
1	A	340	GLN
1	A	482	ASN
1	A	501	GLN
1	A	539	ASN
1	A	606	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	GNP	A	702	2	28,34,34	3.45	9 (32%)	30,54,54	2.36	10 (33%)

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	GNP	A	702	2	-	7/17/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GNP	C4-N9	-12.87	1.30	1.47
3	A	702	GNP	PB-O1B	8.43	1.59	1.46
3	A	702	GNP	C5-C6	-5.39	1.43	1.52
3	A	702	GNP	C8-N9	-4.30	1.30	1.45
3	A	702	GNP	PG-O1G	-3.03	1.41	1.46
3	A	702	GNP	PB-O2B	-2.73	1.49	1.56
3	A	702	GNP	PB-N3B	2.46	1.69	1.63
3	A	702	GNP	PG-O2G	-2.40	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GNP	C2-N1	-2.02	1.36	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	GNP	O2B-PB-O1B	7.20	125.02	109.92
3	A	702	GNP	O1B-PB-N3B	-5.38	103.84	111.77
3	A	702	GNP	O3G-PG-O1G	-3.88	103.71	113.45
3	A	702	GNP	C4-C5-N7	2.86	106.24	102.46
3	A	702	GNP	O2A-PA-O1A	2.66	125.39	112.24
3	A	702	GNP	C2'-C3'-C4'	2.58	107.65	102.64
3	A	702	GNP	O5'-PA-O1A	-2.58	99.00	109.07
3	A	702	GNP	C4'-O4'-C1'	2.52	115.03	109.47
3	A	702	GNP	PA-O3A-PB	-2.11	125.19	132.62
3	A	702	GNP	O2B-PB-O3A	2.10	111.64	104.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	GNP	PA-O3A-PB-O1B
3	A	702	GNP	PA-O3A-PB-O2B
3	A	702	GNP	C2'-C1'-N9-C8
3	A	702	GNP	O4'-C4'-C5'-O5'
3	A	702	GNP	C3'-C4'-C5'-O5'
3	A	702	GNP	C5'-O5'-PA-O3A
3	A	702	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

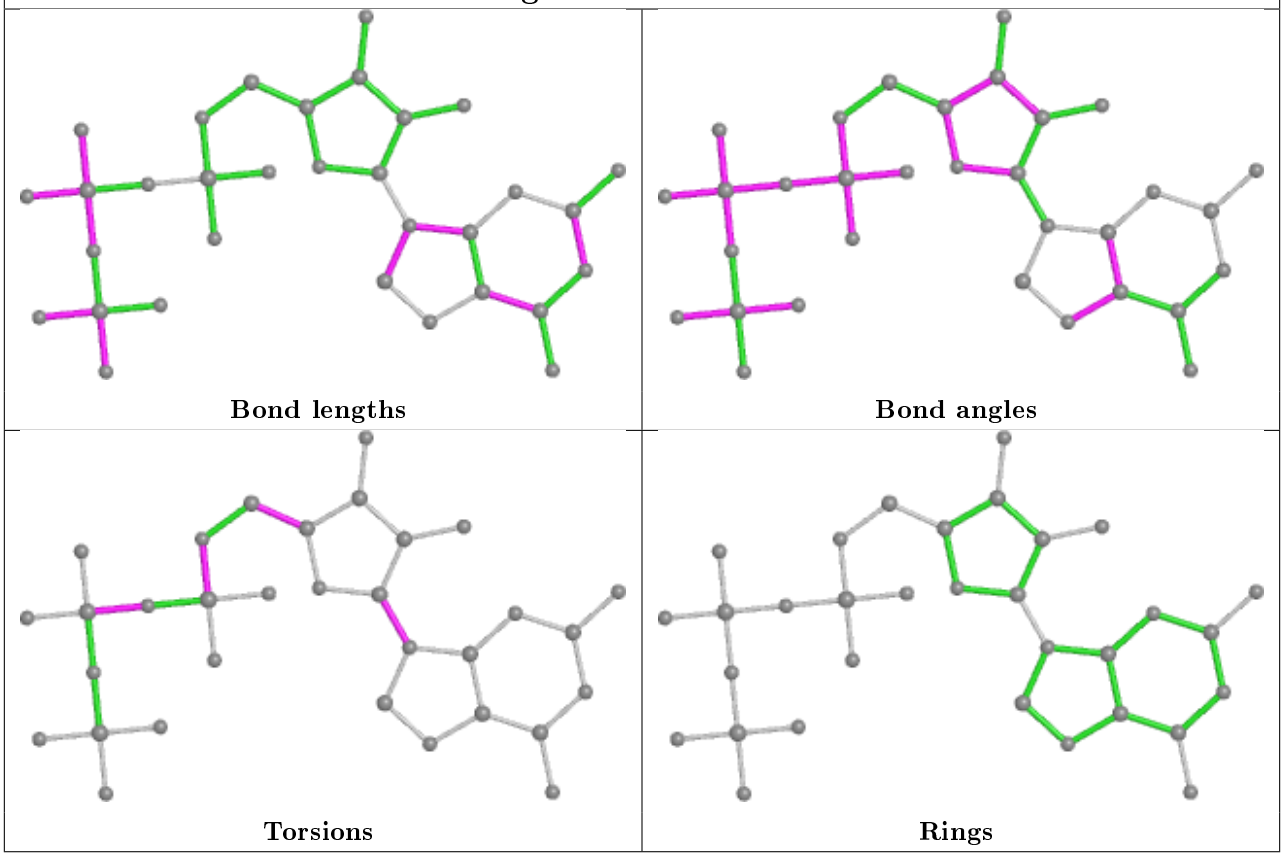
1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	GNP	8	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 GNP A 702



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	656/692 (94%)	0.66	80 (12%) 4 3	30, 84, 186, 256	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	ILE	26.4
1	A	679	TYR	14.8
1	A	591	LEU	10.9
1	A	668	LEU	10.7
1	A	603	ALA	10.3
1	A	601	ALA	10.3
1	A	605	GLN	9.8
1	A	590	TYR	8.9
1	A	602	VAL	8.3
1	A	683	LYS	7.9
1	A	685	SER	7.9
1	A	592	ASN	7.5
1	A	649	ASP	7.2
1	A	672	LYS	7.1
1	A	665	LEU	6.5
1	A	551	TRP	6.5
1	A	612	PRO	6.3
1	A	661	GLU	6.1
1	A	614	LEU	5.6
1	A	667	VAL	4.9
1	A	191	THR	4.6
1	A	589	LEU	4.5
1	A	530	PHE	4.4
1	A	582	ASP	4.4
1	A	598	LYS	4.4
1	A	527	GLY	4.3
1	A	686	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	634	SER	4.3
1	A	610	VAL	4.2
1	A	586	LEU	4.2
1	A	338	LYS	4.2
1	A	515	VAL	4.2
1	A	599	THR	4.1
1	A	594	GLN	4.0
1	A	629	TYR	3.8
1	A	615	THR	3.8
1	A	608	LEU	3.8
1	A	648	ASP	3.6
1	A	681	GLU	3.5
1	A	669	ALA	3.5
1	A	579	PHE	3.4
1	A	651	GLU	3.4
1	A	505	GLY	3.4
1	A	650	GLU	3.3
1	A	684	ARG	3.3
1	A	574	ARG	3.2
1	A	504	LEU	3.2
1	A	585	GLY	3.2
1	A	596	LEU	3.2
1	A	627	PRO	3.1
1	A	578	LYS	3.1
1	A	678	LYS	3.1
1	A	676	ASP	3.0
1	A	529	ASP	3.0
1	A	625	ILE	2.9
1	A	607	ALA	2.9
1	A	609	GLN	2.8
1	A	583	GLU	2.8
1	A	499	SER	2.7
1	A	600	PHE	2.7
1	A	286	HIS	2.6
1	A	662	GLN	2.6
1	A	588	LYS	2.5
1	A	655	PHE	2.5
1	A	604	LYS	2.4
1	A	432	VAL	2.4
1	A	511	THR	2.3
1	A	554	PHE	2.3
1	A	626	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	478	VAL	2.2
1	A	343	PHE	2.2
1	A	632	PHE	2.2
1	A	541	GLN	2.2
1	A	637	ARG	2.2
1	A	420	LEU	2.1
1	A	671	PHE	2.1
1	A	523	TYR	2.1
1	A	633	ASP	2.0
1	A	494	ALA	2.0
1	A	352	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

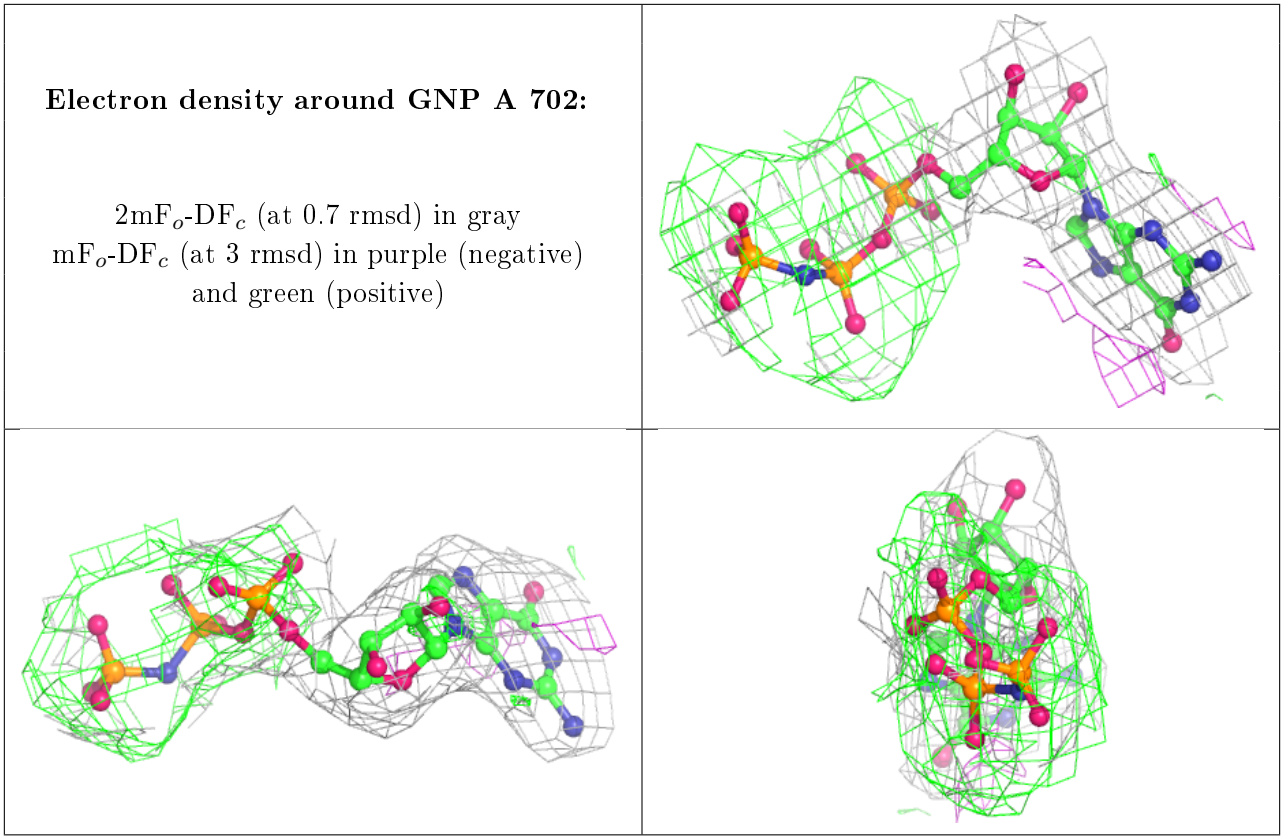
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	A	701	1/1	0.75	0.35	38,38,38,38	0
3	GNP	A	702	32/32	0.82	0.40	16,28,40,47	12

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 GNP A 702:

$2mF_o$-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.