



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:43 am BST

PDB ID : 2NPF
Title : Structure of eEF2 in complex with moriniafungin
Authors : Soe, R.; Mosley, R.T.; Andersen, G.R.
Deposited on : 2006-10-27
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

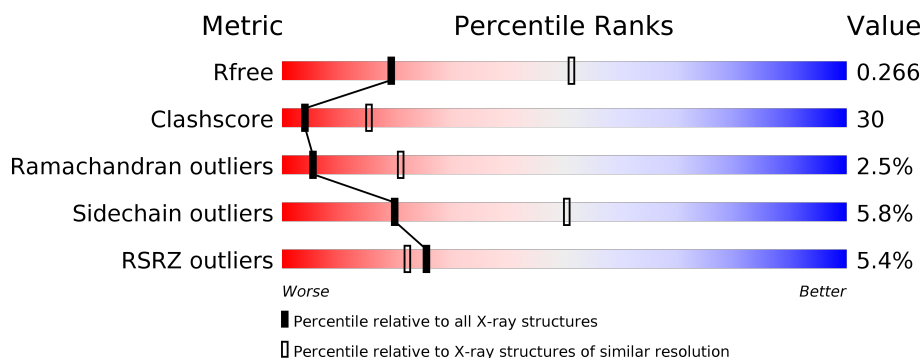
1 Overall quality at a glance

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	842	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>40%</div> <div>• •</div> </div> </div>
1	B	842	<div> <div>7%</div> <div> <div></div> <div>47%</div> <div>46%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

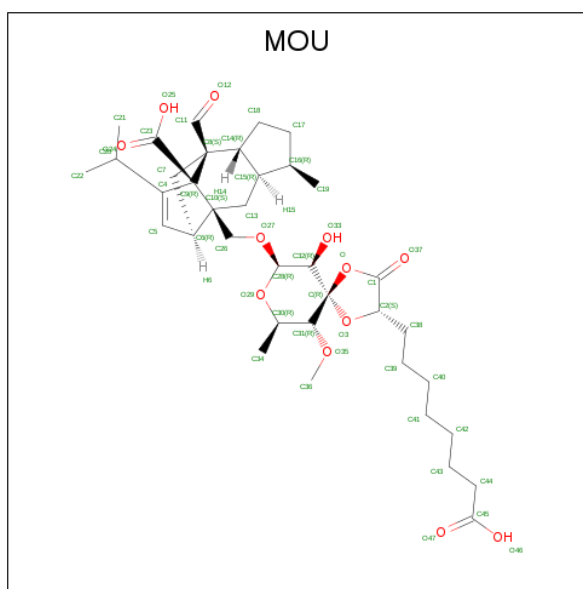
There are 3 unique types of molecules in this entry. The entry contains 12885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6397	4070	1092	1205	30			
1	B	813	Total	C	N	O	S	0	0	0
			6334	4032	1078	1194	30			

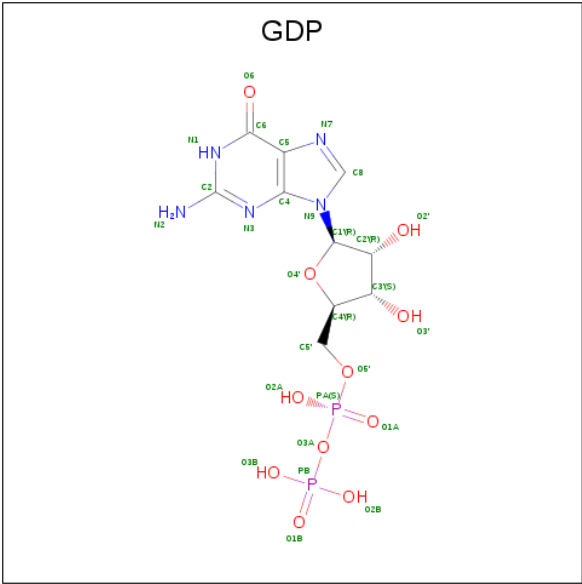
- Molecule 2 is (1S,4R,5R,9S,11S)-2-({[(2S,5R,6R,7R,9S,10R)-2-(7-CARBOXYHEPTYL)-6-HYDROXY-10-METHOXY-9-METHYL-3-OXO-1,4,8-TRIOXASPIRO[4.5]DEC-7-YL]OXY}METHYL)-9-FORMYL-13-ISOPROPYL-5-METHYLTETRACYCLO[7.4.0.0.2,11.04.8]TRIDEC-12-ENE-1-CARBOXYLIC ACID (three-letter code: MOU) (formula: C₃₇H₅₄O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			49	37	12		
2	B	1	Total	C	O	0	0
			49	37	12		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:

C₁₀H₁₅N₅O₁₁P₂).

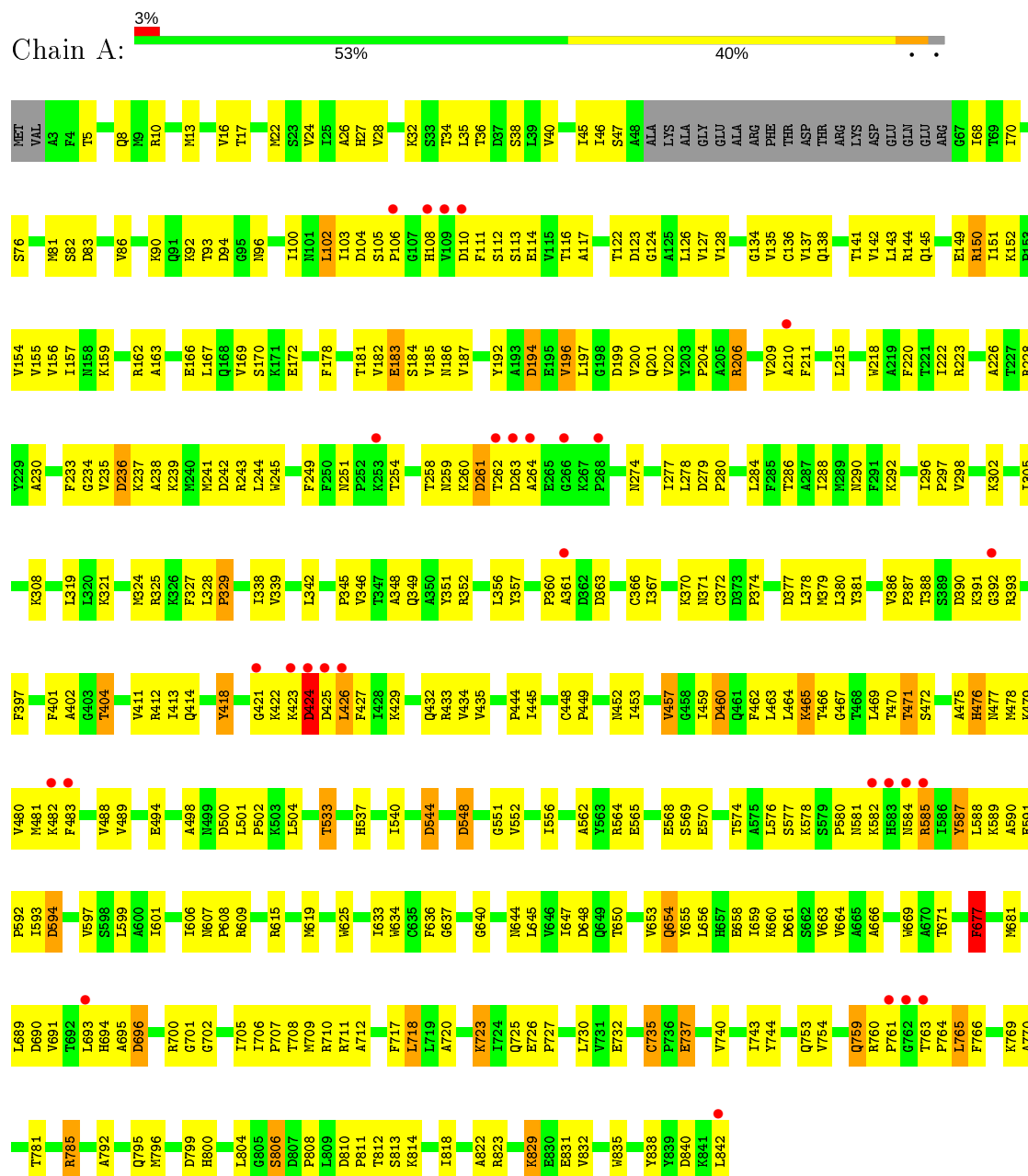


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

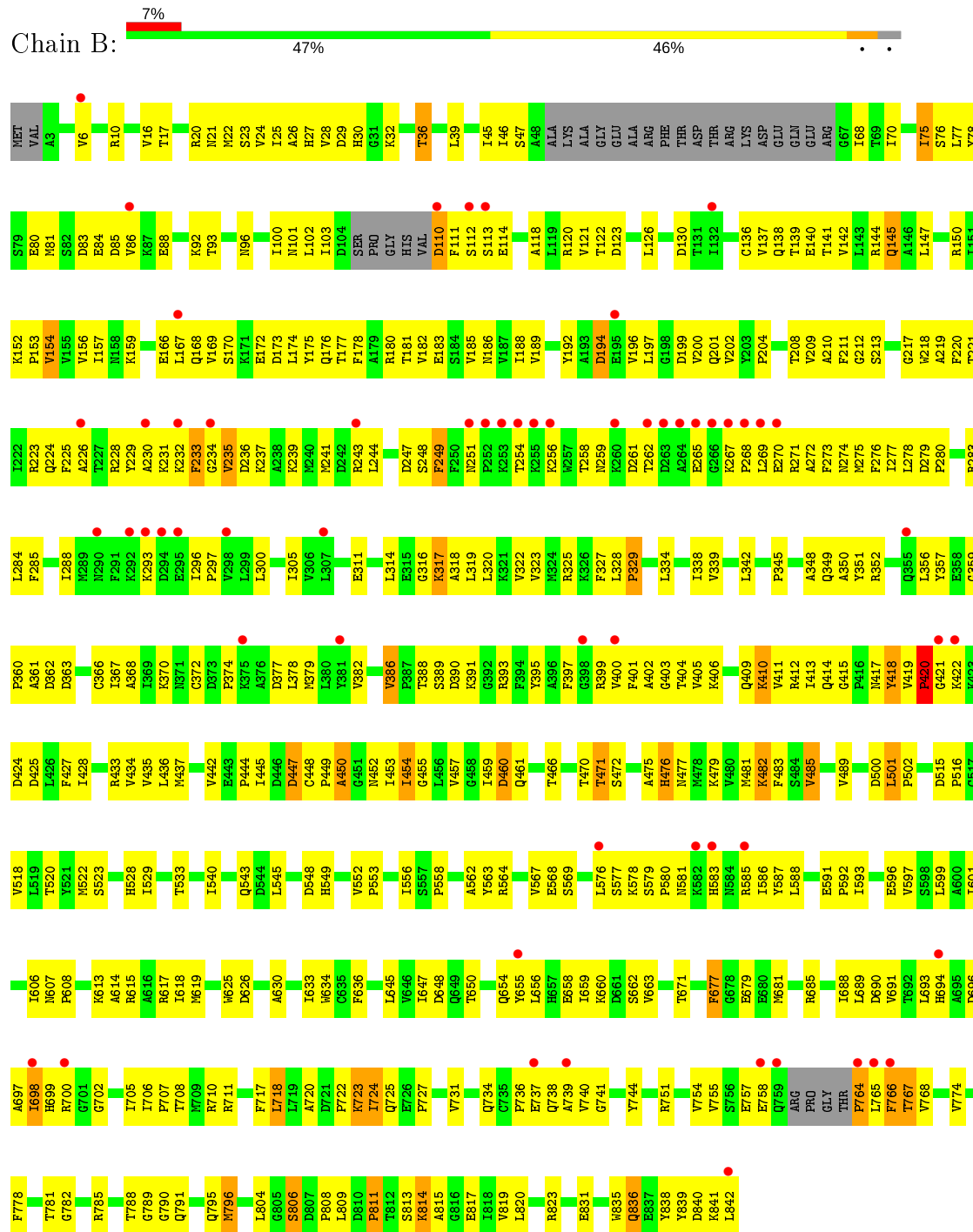
3 Residue-property plots

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

• Molecule 1: Elongation factor 2



• Molecule 1: Elongation factor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.97Å 159.12Å 112.14Å 90.00° 97.83° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 33.70 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.00-2.90) 99.6 (33.70-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.271 0.226 , 0.266	Depositor DCC
R_{free} test set	1162 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12885	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/6521	0.70	0/8831
1	B	0.40	1/6453 (0.0%)	0.74	6/8733 (0.1%)
All	All	0.42	1/12974 (0.0%)	0.72	6/17564 (0.0%)

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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	764	PRO	C-N	-8.45	1.14	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	764	PRO	O-C-N	-22.15	87.26	122.70
1	B	764	PRO	C-N-CA	15.74	161.05	121.70
1	B	764	PRO	CA-C-N	14.56	149.24	117.20
1	B	764	PRO	CA-N-CD	-8.86	99.09	111.50
1	B	767	THR	N-CA-C	8.33	133.50	111.00
1	B	766	PHE	O-C-N	5.12	130.90	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	764	PRO	Mainchain,Peptide

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	6397	0	6465	354	0
1	B	6334	0	6402	424	0
2	A	49	0	52	1	0
2	B	49	0	52	1	0
3	A	28	0	12	4	0
3	B	28	0	12	2	0
All	All	12885	0	12995	778	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 30.

All (778) 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:764:PRO:O	1:A:765:LEU:CG	1.75	1.32
1:B:737:GLU:HA	1:B:766:PHE:HZ	1.04	1.19
1:B:737:GLU:HA	1:B:766:PHE:CZ	1.80	1.17
1:B:296:ILE:HG13	1:B:297:PRO:HD3	1.27	1.15
1:B:360:PRO:HG2	1:B:363:ASP:HB2	1.40	1.03
1:B:694:HIS:H	1:B:700:ARG:HD3	1.21	1.00
1:A:463:LEU:HD21	1:A:467:GLY:HA3	1.44	1.00
1:A:27:HIS:CD2	1:A:28:VAL:H	1.80	0.98
1:A:764:PRO:O	1:A:765:LEU:HG	0.81	0.98
1:B:482:LYS:HD2	1:B:482:LYS:H	1.27	0.97
1:A:360:PRO:HG2	1:A:363:ASP:HB2	1.47	0.97
1:A:764:PRO:C	1:A:765:LEU:HG	1.86	0.95
1:B:754:VAL:HG11	1:B:757:GLU:OE2	1.67	0.95
1:B:196:VAL:HG13	1:B:197:LEU:HD13	1.48	0.94
1:A:27:HIS:HD2	1:A:28:VAL:H	0.97	0.93
1:A:114:GLU:HA	1:A:481:MET:HE1	1.49	0.93
1:B:734:GLN:HE21	1:B:767:THR:CG2	1.83	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.52	0.90
1:A:223:ARG:HA	1:A:241:MET:HE2	1.52	0.90
1:B:296:ILE:CG1	1:B:297:PRO:HD3	2.04	0.87
1:A:711:ARG:NH1	1:A:838:TYR:HA	1.90	0.86
1:B:740:VAL:HG21	1:B:766:PHE:CE1	2.10	0.86
1:A:655:TYR:HB3	1:A:658:GLU:HG3	1.55	0.86
1:B:234:GLY:O	1:B:235:VAL:HG23	1.75	0.86
1:A:759:GLN:HG3	1:A:760:ARG:N	1.89	0.85
1:B:578:LYS:HG2	1:B:840:ASP:OD2	1.77	0.85
1:B:32:LYS:O	1:B:36:THR:HG22	1.77	0.84
1:B:110:ASP:O	1:B:789:GLY:HA3	1.78	0.83
1:B:650:THR:HG22	1:B:690:ASP:HA	1.58	0.83
1:B:284:LEU:O	1:B:288:ILE:HD13	1.79	0.83
1:B:10:ARG:HH12	1:B:448:CYS:HA	1.43	0.82
1:B:489:VAL:HG12	1:B:781:THR:HG21	1.58	0.82
1:B:836:GLN:H	1:B:836:GLN:NE2	1.77	0.82
1:B:740:VAL:HG21	1:B:766:PHE:CZ	2.15	0.82
1:A:740:VAL:HA	1:A:743:ILE:HD12	1.61	0.82
1:A:829:LYS:HA	1:A:829:LYS:HE3	1.62	0.81
1:A:27:HIS:CD2	1:A:28:VAL:N	2.47	0.81
1:A:763:THR:O	1:A:763:THR:HG22	1.81	0.81
1:B:740:VAL:HG12	1:B:744:TYR:HE2	1.46	0.80
1:B:706:ILE:HB	1:B:707:PRO:HD3	1.63	0.80
1:B:737:GLU:CA	1:B:766:PHE:CZ	2.63	0.79
1:A:576:LEU:HD11	1:A:585:ARG:HD2	1.63	0.79
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.63	0.79
1:A:781:THR:HG22	2:A:901:MOU:O46	1.82	0.79
1:B:27:HIS:HB3	1:B:30:HIS:ND1	1.96	0.79
1:A:27:HIS:HD2	1:A:28:VAL:N	1.78	0.78
1:A:764:PRO:HD2	1:A:765:LEU:H	1.46	0.78
1:B:417:ASN:HD21	1:B:483:PHE:HZ	1.30	0.78
1:A:489:VAL:HG13	1:A:781:THR:HG21	1.66	0.78
1:B:296:ILE:HG13	1:B:297:PRO:CD	2.12	0.78
1:B:156:VAL:HG22	1:B:210:ALA:HB3	1.66	0.78
1:A:150:ARG:N	1:A:150:ARG:HD3	1.98	0.78
1:B:737:GLU:HB3	1:B:766:PHE:HE2	1.49	0.78
1:B:279:ASP:HB3	1:B:280:PRO:HD3	1.65	0.77
1:B:597:VAL:O	1:B:601:ILE:HG12	1.85	0.77
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.50	0.77
1:B:454:ILE:HD13	1:B:455:GLY:N	1.99	0.77
1:A:46:ILE:HG22	1:A:47:SER:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:ARG:HG2	1:A:764:PRO:HG2	1.66	0.77
1:B:270:GLU:HG2	1:B:275:MET:CE	2.15	0.77
1:B:694:HIS:N	1:B:700:ARG:HD3	1.99	0.76
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.21	0.76
1:B:734:GLN:HE21	1:B:767:THR:HG21	1.50	0.76
1:B:613:LYS:O	1:B:617:ARG:HG3	1.86	0.75
1:A:28:VAL:HG23	1:A:138:GLN:HE22	1.52	0.75
1:B:577:SER:HA	1:B:840:ASP:HB2	1.69	0.75
1:A:533:THR:HB	1:A:537:HIS:ND1	2.00	0.75
1:B:472:SER:HB3	1:B:475:ALA:HB2	1.68	0.75
1:B:737:GLU:HB3	1:B:766:PHE:CE2	2.23	0.74
1:B:744:TYR:OH	1:B:757:GLU:HG2	1.88	0.73
1:A:204:PRO:O	1:A:222:ILE:HD13	1.87	0.73
1:B:781:THR:HG22	2:B:1901:MOU:O46	1.87	0.73
1:B:243:ARG:HD3	1:B:248:SER:OG	1.89	0.73
1:A:199:ASP:OD1	1:A:201:GLN:HG3	1.87	0.73
1:A:760:ARG:HH21	1:A:761:PRO:HG2	1.52	0.73
1:A:615:ARG:HG2	1:A:619:MET:CE	2.20	0.72
1:B:142:VAL:HA	1:B:145:GLN:CD	2.09	0.72
1:B:334:LEU:O	1:B:338:ILE:HG12	1.90	0.72
1:A:32:LYS:O	1:A:36:THR:HG23	1.89	0.72
1:A:659:ILE:HD13	1:A:693:LEU:HD21	1.72	0.72
1:A:17:THR:HG21	1:A:92:LYS:HG3	1.72	0.72
1:B:10:ARG:NH1	1:B:449:PRO:HD3	2.05	0.72
1:B:418:TYR:O	1:B:419:VAL:HG23	1.88	0.72
1:B:576:LEU:CD2	1:B:842:LEU:HG	2.20	0.71
1:B:634:TRP:CZ3	1:B:660:LYS:HA	2.24	0.71
1:B:30:HIS:CD2	1:B:130:ASP:HB2	2.24	0.71
1:B:410:LYS:H	1:B:410:LYS:HD2	1.55	0.71
1:A:27:HIS:ND1	1:A:136:CYS:SG	2.59	0.71
1:B:27:HIS:ND1	1:B:138:GLN:HB3	2.05	0.71
1:A:489:VAL:CG1	1:A:781:THR:HG21	2.21	0.70
1:A:418:TYR:CE1	1:A:426:LEU:HG	2.27	0.70
1:A:10:ARG:NH2	1:A:449:PRO:HD3	2.06	0.70
1:B:231:LYS:C	1:B:233:PHE:H	1.93	0.70
1:A:277:ILE:O	1:A:280:PRO:HD2	1.92	0.70
1:B:176:GLN:O	1:B:180:ARG:HG3	1.92	0.70
1:B:348:ALA:HA	1:B:351:TYR:CE2	2.26	0.70
1:A:760:ARG:NE	1:A:761:PRO:HD2	2.06	0.69
1:B:417:ASN:HB2	1:B:425:ASP:OD2	1.92	0.69
1:A:222:ILE:HD12	1:A:222:ILE:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LYS:C	1:A:424:ASP:N	2.45	0.69
1:B:25:ILE:HG23	1:B:142:VAL:HG11	1.74	0.69
1:A:13:MET:HG2	1:A:452:ASN:ND2	2.06	0.69
1:A:585:ARG:HH22	1:A:842:LEU:C	1.95	0.69
1:A:34:THR:HG23	3:A:902:GDP:O1A	1.92	0.69
1:B:126:LEU:HD11	1:B:156:VAL:HG23	1.75	0.68
1:B:70:ILE:HG22	1:B:388:THR:HG22	1.74	0.68
1:A:46:ILE:HG22	1:A:47:SER:N	2.07	0.68
1:B:249:PHE:N	1:B:249:PHE:HD1	1.90	0.68
1:B:806:SER:HB3	1:B:813:SER:HB2	1.76	0.68
1:A:126:LEU:HD11	1:A:156:VAL:HG23	1.76	0.68
1:B:172:GLU:HA	1:B:274:ASN:HD21	1.56	0.68
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.76	0.68
1:B:140:GLU:O	1:B:144:ARG:HG3	1.93	0.68
1:A:186:ASN:OD1	1:A:201:GLN:HB3	1.94	0.67
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.76	0.67
1:A:422:LYS:N	1:A:422:LYS:HD2	2.09	0.67
1:B:226:ALA:O	1:B:230:ALA:HB2	1.95	0.67
1:B:285:PHE:CE1	1:B:320:LEU:HD21	2.28	0.67
1:B:239:LYS:HE3	1:B:243:ARG:HE	1.60	0.67
1:A:137:VAL:HG23	1:A:138:GLN:H	1.60	0.67
1:B:45:ILE:O	1:B:46:ILE:HD13	1.94	0.67
1:A:463:LEU:O	1:A:464:LEU:HD23	1.95	0.66
1:B:379:MET:HB2	1:B:402:ALA:HB3	1.77	0.66
1:B:694:HIS:H	1:B:700:ARG:CD	2.03	0.66
1:B:194:ASP:HB3	1:B:196:VAL:HG12	1.77	0.66
1:B:10:ARG:CZ	1:B:449:PRO:HD3	2.25	0.66
1:A:799:ASP:OD1	1:A:800:HIS:HD2	1.78	0.66
1:B:636:PHE:CE1	1:B:645:LEU:HD21	2.31	0.66
1:B:694:HIS:HB3	1:B:700:ARG:HD3	1.77	0.66
1:A:82:SER:O	1:A:86:VAL:HG23	1.96	0.66
1:B:249:PHE:N	1:B:249:PHE:CD1	2.61	0.66
1:B:249:PHE:CE2	1:B:261:ASP:HA	2.31	0.66
1:B:723:LYS:HA	1:B:808:PRO:HG2	1.78	0.65
1:B:220:PHE:HB3	1:B:328:LEU:HD13	1.77	0.65
1:B:377:ASP:HB3	1:B:472:SER:HB2	1.79	0.65
1:B:174:LEU:HD23	1:B:278:LEU:HD22	1.79	0.65
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.27	0.65
1:B:345:PRO:O	1:B:349:GLN:HG3	1.97	0.65
1:B:587:TYR:HE1	1:B:842:LEU:HD11	1.60	0.65
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.31	0.65
1:B:296:ILE:O	1:B:300:LEU:HD13	1.97	0.65
1:A:422:LYS:HB2	1:A:424:ASP:OD2	1.97	0.64
1:A:763:THR:N	1:A:764:PRO:HD3	2.13	0.64
1:B:489:VAL:CG1	1:B:781:THR:HG21	2.28	0.64
1:A:144:ARG:HD2	1:A:192:TYR:CE2	2.32	0.64
1:A:764:PRO:HD2	1:A:765:LEU:N	2.12	0.64
1:B:659:ILE:HD13	1:B:693:LEU:HD21	1.79	0.64
1:A:754:VAL:HA	1:A:770:ALA:HB2	1.79	0.64
1:A:706:ILE:H	1:A:706:ILE:HD12	1.61	0.64
1:B:169:VAL:HG12	1:B:170:SER:O	1.97	0.64
1:A:764:PRO:CD	1:A:765:LEU:H	2.11	0.64
1:A:823:ARG:HE	1:A:832:VAL:HG22	1.63	0.64
1:A:114:GLU:HA	1:A:481:MET:CE	2.27	0.64
1:A:615:ARG:HG2	1:A:619:MET:HE2	1.80	0.64
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.63	0.64
1:B:648:ASP:C	1:B:648:ASP:OD2	2.36	0.64
1:B:737:GLU:CA	1:B:766:PHE:CE2	2.81	0.64
1:B:228:ARG:HG2	1:B:232:LYS:HE3	1.80	0.64
1:B:248:SER:C	1:B:249:PHE:HD1	2.01	0.64
1:B:655:TYR:CB	1:B:700:ARG:HH22	2.11	0.64
1:A:568:GLU:HB2	1:A:723:LYS:HD3	1.80	0.64
1:B:126:LEU:HD11	1:B:156:VAL:CG2	2.28	0.64
1:B:615:ARG:HH11	1:B:615:ARG:HB2	1.63	0.63
1:B:711:ARG:CZ	1:B:838:TYR:HA	2.29	0.63
1:B:10:ARG:NH1	1:B:448:CYS:HA	2.12	0.63
1:B:120:ARG:HH12	1:B:481:MET:CE	2.12	0.63
1:A:141:THR:O	1:A:145:GLN:HG3	1.98	0.63
1:A:607:ASN:OD1	1:A:609:ARG:HG2	1.98	0.63
1:B:217:GLY:HA3	1:B:325:ARG:NH1	2.12	0.63
1:A:434:VAL:O	1:A:445:ILE:HG22	1.99	0.63
1:B:399:ARG:HD3	1:B:401:PHE:CZ	2.34	0.63
1:A:597:VAL:O	1:A:601:ILE:HG12	1.99	0.62
1:B:169:VAL:HG12	1:B:170:SER:N	2.14	0.62
1:B:435:VAL:HG12	1:B:444:PRO:HA	1.81	0.62
1:A:404:THR:HB	1:A:449:PRO:HA	1.80	0.62
1:B:740:VAL:HG21	1:B:766:PHE:HE1	1.65	0.62
1:A:28:VAL:HG23	1:A:138:GLN:NE2	2.14	0.62
1:A:429:LYS:HG2	1:A:462:PHE:CE2	2.34	0.62
1:A:464:LEU:O	1:A:465:LYS:HB2	1.99	0.62
1:A:45:ILE:HD12	1:A:76:SER:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:ARG:HG2	1:B:619:MET:CE	2.30	0.62
1:A:829:LYS:CE	1:A:829:LYS:HA	2.27	0.62
1:A:422:LYS:C	1:A:424:ASP:H	2.02	0.62
1:B:809:LEU:O	1:B:811:PRO:HD3	2.00	0.62
1:B:552:VAL:HG13	1:B:553:PRO:HD2	1.82	0.62
1:B:86:VAL:HG13	1:B:93:THR:HG21	1.80	0.62
1:A:569:SER:O	1:A:720:ALA:HB1	2.00	0.61
1:A:735:CYS:HB2	1:A:792:ALA:HA	1.81	0.61
1:B:482:LYS:H	1:B:482:LYS:CD	2.08	0.61
1:B:419:VAL:HG13	1:B:420:PRO:HD2	1.83	0.61
1:B:576:LEU:HD12	1:B:586:ILE:O	2.00	0.61
1:B:17:THR:HB	1:B:92:LYS:O	2.01	0.61
1:B:226:ALA:HB2	1:B:244:LEU:HD12	1.83	0.61
1:B:568:GLU:HB2	1:B:723:LYS:HD3	1.81	0.61
1:A:634:TRP:CZ3	1:A:660:LYS:HA	2.36	0.61
1:B:251:ASN:HB3	1:B:254:THR:OG1	2.00	0.61
1:A:113:SER:O	1:A:116:THR:HG22	2.00	0.60
1:B:417:ASN:ND2	1:B:483:PHE:HZ	1.99	0.60
1:A:634:TRP:CE3	1:A:660:LYS:HG3	2.36	0.60
1:B:489:VAL:HG12	1:B:781:THR:CG2	2.31	0.60
1:B:734:GLN:NE2	1:B:767:THR:CG2	2.59	0.60
1:B:152:LYS:HG3	1:B:200:VAL:HG23	1.84	0.60
1:B:482:LYS:HD2	1:B:482:LYS:N	2.07	0.60
1:B:142:VAL:HA	1:B:145:GLN:NE2	2.15	0.60
1:B:154:VAL:HG22	1:B:342:LEU:HD21	1.83	0.60
1:B:421:GLY:O	1:B:422:LYS:HD3	2.01	0.60
1:A:325:ARG:O	1:A:329:PRO:HG3	2.01	0.60
1:A:413:ILE:HD13	1:A:459:ILE:HG23	1.83	0.60
1:A:760:ARG:CG	1:A:764:PRO:HG2	2.32	0.60
1:A:823:ARG:NE	1:A:832:VAL:HG22	2.16	0.60
1:A:345:PRO:O	1:A:349:GLN:HG3	2.02	0.60
1:B:277:ILE:O	1:B:280:PRO:HD2	2.02	0.60
1:B:694:HIS:ND1	1:B:696:ASP:N	2.49	0.59
1:A:806:SER:HB3	1:A:813:SER:HB2	1.83	0.59
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.85	0.59
1:B:186:ASN:OD1	1:B:201:GLN:HB3	2.02	0.59
1:B:734:GLN:HE21	1:B:767:THR:HG22	1.62	0.59
1:A:236:ASP:OD2	1:A:239:LYS:HB3	2.02	0.59
1:B:311:GLU:HA	1:B:314:LEU:HG	1.83	0.59
1:B:389:SER:C	1:B:391:LYS:H	2.05	0.59
1:B:615:ARG:HG2	1:B:619:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:ARG:NH1	1:B:615:ARG:HB2	2.18	0.59
1:B:84:GLU:HG3	1:B:85:ASP:N	2.18	0.59
1:A:363:ASP:O	1:A:367:ILE:HG12	2.03	0.59
1:A:760:ARG:HG2	1:A:764:PRO:CG	2.32	0.59
1:A:202:VAL:HG12	1:A:209:VAL:HG23	1.85	0.59
1:A:260:LYS:HE2	1:A:260:LYS:HA	1.83	0.59
1:A:615:ARG:HG2	1:A:619:MET:HE1	1.84	0.59
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.85	0.59
1:A:423:LYS:O	1:A:425:ASP:N	2.35	0.59
1:B:361:ALA:HA	1:B:366:CYS:SG	2.43	0.59
1:B:169:VAL:HG13	1:B:173:ASP:HB2	1.85	0.59
1:B:614:ALA:O	1:B:618:ILE:HG12	2.02	0.59
1:A:13:MET:HG2	1:A:452:ASN:HD22	1.67	0.58
1:B:377:ASP:CB	1:B:472:SER:HB2	2.33	0.58
1:B:270:GLU:HG2	1:B:275:MET:SD	2.44	0.58
1:B:694:HIS:HB3	1:B:700:ARG:CD	2.32	0.58
1:B:738:GLN:CG	1:B:739:ALA:N	2.65	0.58
1:A:16:VAL:O	1:A:345:PRO:HD2	2.03	0.58
1:A:744:TYR:CE1	1:A:754:VAL:HG21	2.38	0.58
1:A:202:VAL:HG12	1:A:209:VAL:CG2	2.34	0.58
1:A:753:GLN:O	1:A:770:ALA:HB1	2.04	0.58
1:B:10:ARG:NH2	1:B:449:PRO:HD3	2.18	0.58
1:B:70:ILE:HG22	1:B:388:THR:CG2	2.33	0.58
1:B:727:PRO:HG2	1:B:774:VAL:HB	1.84	0.58
1:A:263:ASP:CG	1:A:264:ALA:H	2.07	0.58
1:B:100:ILE:HD12	1:B:338:ILE:HG21	1.86	0.58
1:B:275:MET:HA	1:B:275:MET:CE	2.34	0.58
1:B:576:LEU:HD21	1:B:585:ARG:CZ	2.34	0.57
1:A:222:ILE:N	1:A:222:ILE:HD12	2.19	0.57
1:B:27:HIS:HD2	1:B:28:VAL:O	1.87	0.57
1:B:806:SER:OG	1:B:814:LYS:HG2	2.05	0.57
1:A:500:ASP:HB3	1:A:552:VAL:HG21	1.85	0.57
1:A:737:GLU:OE2	1:A:763:THR:HG21	2.05	0.57
1:A:137:VAL:HG23	1:A:138:GLN:N	2.20	0.57
1:B:418:TYR:HB2	1:B:425:ASP:CB	2.34	0.57
1:B:785:ARG:HB2	1:B:790:GLY:HA2	1.85	0.57
1:B:249:PHE:HB2	1:B:258:THR:HG23	1.86	0.57
1:B:418:TYR:HB2	1:B:425:ASP:HB3	1.87	0.57
1:B:177:THR:HG23	1:B:180:ARG:HH21	1.70	0.57
1:B:20:ARG:HB2	1:B:100:ILE:HD13	1.85	0.56
1:A:648:ASP:C	1:A:648:ASP:OD2	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.87	0.56
1:B:636:PHE:CD1	1:B:645:LEU:HD21	2.40	0.56
1:A:24:VAL:HG23	1:A:102:LEU:HD11	1.87	0.56
1:A:155:VAL:HG12	1:A:156:VAL:N	2.19	0.56
1:B:181:THR:O	1:B:185:VAL:HG23	2.05	0.56
1:B:819:VAL:O	1:B:823:ARG:HG3	2.04	0.56
1:B:26:ALA:HB3	1:B:32:LYS:HB2	1.87	0.56
1:A:422:LYS:O	1:A:424:ASP:HB2	2.06	0.56
1:A:110:ASP:O	1:A:112:SER:N	2.38	0.56
1:B:619:MET:HE3	1:B:630:ALA:HA	1.87	0.56
1:B:111:PHE:HA	1:B:789:GLY:O	2.06	0.56
1:B:223:ARG:NH1	1:B:223:ARG:HG2	2.18	0.56
1:B:724:ILE:H	1:B:724:ILE:HD13	1.70	0.56
1:B:736:PRO:O	1:B:740:VAL:HG23	2.05	0.56
1:B:417:ASN:ND2	1:B:483:PHE:CZ	2.70	0.56
1:B:150:ARG:NH2	1:B:196:VAL:HG11	2.21	0.56
1:B:10:ARG:HH12	1:B:448:CYS:CA	2.17	0.56
1:B:213:SER:HB3	1:B:218:TRP:NE1	2.21	0.55
1:B:169:VAL:CG1	1:B:173:ASP:HB2	2.36	0.55
1:B:608:PRO:HG3	1:B:636:PHE:CD2	2.41	0.55
1:A:433:ARG:HB2	1:A:457:VAL:HG22	1.89	0.55
1:A:381:TYR:HE1	1:A:480:VAL:HG12	1.71	0.55
1:A:588:LEU:HD12	1:A:588:LEU:C	2.27	0.55
1:B:248:SER:C	1:B:249:PHE:CD1	2.80	0.55
1:A:159:LYS:HG2	3:A:902:GDP:C6	2.42	0.55
1:B:424:ASP:O	1:B:425:ASP:HB2	2.05	0.55
1:A:412:ARG:NH2	1:A:418:TYR:OH	2.39	0.55
1:B:327:PHE:O	1:B:328:LEU:HD23	2.07	0.55
1:A:28:VAL:CG2	1:A:138:GLN:HE22	2.19	0.55
1:B:25:ILE:HG23	1:B:142:VAL:CG1	2.35	0.55
1:B:691:VAL:HG12	1:B:693:LEU:HG	1.87	0.55
1:B:615:ARG:O	1:B:619:MET:HG3	2.07	0.55
1:B:630:ALA:O	1:B:633:ILE:HG12	2.07	0.55
1:A:200:VAL:HG22	1:A:200:VAL:O	2.08	0.55
1:B:196:VAL:HG13	1:B:197:LEU:CD1	2.29	0.55
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.88	0.54
1:A:760:ARG:CG	1:A:764:PRO:CD	2.85	0.54
1:A:284:LEU:HD13	1:A:324:MET:CE	2.37	0.54
1:A:551:GLY:O	1:A:552:VAL:HG23	2.06	0.54
1:A:578:LYS:HG2	1:A:840:ASP:OD2	2.08	0.54
1:B:737:GLU:CB	1:B:766:PHE:CE2	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:HA	1:A:274:ASN:ND2	2.22	0.54
1:A:421:GLY:C	1:A:422:LYS:HD2	2.28	0.54
1:A:799:ASP:OD1	1:A:800:HIS:CD2	2.60	0.54
1:B:434:VAL:HG12	1:B:445:ILE:CG2	2.37	0.54
1:A:327:PHE:O	1:A:328:LEU:HD23	2.07	0.54
1:B:218:TRP:HA	1:B:328:LEU:O	2.08	0.54
1:B:200:VAL:O	1:B:200:VAL:HG22	2.07	0.54
1:B:16:VAL:O	1:B:345:PRO:HD2	2.07	0.54
1:B:758:GLU:O	1:B:766:PHE:HB2	2.07	0.54
1:A:706:ILE:HB	1:A:707:PRO:CD	2.33	0.53
1:B:141:THR:O	1:B:145:GLN:HG3	2.08	0.53
1:B:711:ARG:NH1	1:B:838:TYR:HA	2.23	0.53
1:A:760:ARG:HG2	1:A:764:PRO:CD	2.38	0.53
1:A:718:LEU:HB3	1:A:835:TRP:HB3	1.90	0.53
1:B:228:ARG:HG2	1:B:232:LYS:CE	2.38	0.53
1:A:194:ASP:HB2	1:A:197:LEU:HD13	1.89	0.53
1:A:163:ALA:O	1:A:169:VAL:HG23	2.08	0.53
1:B:737:GLU:CB	1:B:766:PHE:HE2	2.21	0.53
1:B:147:LEU:HD11	1:B:189:VAL:HA	1.91	0.53
1:B:29:ASP:HA	3:B:1902:GDP:H5'	1.90	0.53
1:B:413:ILE:HB	1:B:427:PHE:HB2	1.90	0.53
1:A:414:GLN:HB3	1:A:418:TYR:HD2	1.74	0.53
1:A:556:ILE:N	1:A:556:ILE:HD12	2.24	0.53
1:A:581:ASN:O	1:A:582:LYS:HB2	2.09	0.53
1:B:634:TRP:NE1	1:B:648:ASP:HB2	2.23	0.53
1:B:75:ILE:HD12	1:B:75:ILE:N	2.24	0.53
1:B:363:ASP:O	1:B:367:ILE:HG12	2.09	0.53
1:A:162:ARG:HH11	1:A:162:ARG:HG2	1.74	0.53
1:A:418:TYR:HD2	1:A:477:ASN:HD21	1.57	0.53
1:B:229:TYR:HE2	1:B:276:PHE:HB3	1.73	0.53
1:B:86:VAL:HG21	1:B:96:ASN:OD1	2.09	0.53
1:A:763:THR:O	1:A:763:THR:CG2	2.54	0.52
1:B:27:HIS:ND1	1:B:138:GLN:CB	2.72	0.52
1:A:277:ILE:HD12	1:A:277:ILE:N	2.24	0.52
1:A:434:VAL:HG12	1:A:445:ILE:CG2	2.38	0.52
1:A:633:ILE:HG22	1:A:647:ILE:HG13	1.91	0.52
1:B:738:GLN:HG3	1:B:739:ALA:N	2.25	0.52
1:A:116:THR:HG23	1:A:117:ALA:N	2.25	0.52
1:A:251:ASN:HB3	1:A:254:THR:OG1	2.09	0.52
1:A:671:THR:HA	1:A:681:MET:HG3	1.92	0.52
1:A:226:ALA:O	1:A:230:ALA:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:GLU:HG3	1:B:768:VAL:HG22	1.91	0.52
1:A:448:CYS:SG	1:A:452:ASN:HB2	2.49	0.52
1:A:654:GLN:HG2	1:A:655:TYR:CD2	2.44	0.52
1:B:10:ARG:HH12	1:B:449:PRO:HD3	1.74	0.52
1:B:677:PHE:CD2	1:B:677:PHE:N	2.77	0.52
1:B:734:GLN:NE2	1:B:767:THR:HG21	2.23	0.52
1:A:124:GLY:HA3	1:A:342:LEU:HD22	1.91	0.52
1:A:284:LEU:HD13	1:A:324:MET:HE3	1.92	0.52
1:A:459:ILE:HD13	1:A:469:LEU:HD21	1.91	0.52
1:B:175:TYR:HD1	1:B:273:PHE:CD2	2.27	0.52
1:B:434:VAL:HG13	1:B:454:ILE:CD1	2.39	0.52
1:B:10:ARG:NH1	1:B:447:ASP:O	2.43	0.52
1:B:68:ILE:HD13	1:B:390:ASP:OD2	2.10	0.52
1:B:202:VAL:HG12	1:B:209:VAL:CG2	2.39	0.52
1:A:429:LYS:HE2	1:A:462:PHE:CZ	2.45	0.51
1:A:501:LEU:HD23	1:A:501:LEU:O	2.10	0.51
1:A:732:GLU:OE2	1:A:769:LYS:HE2	2.10	0.51
1:B:88:GLU:HG3	1:B:223:ARG:HH21	1.74	0.51
1:B:319:LEU:O	1:B:323:VAL:HG23	2.10	0.51
1:B:405:VAL:HA	1:B:409:GLN:OE1	2.10	0.51
1:B:271:ARG:HH11	1:B:271:ARG:HG3	1.75	0.51
1:B:338:ILE:HG23	1:B:342:LEU:HD12	1.91	0.51
1:B:120:ARG:HH12	1:B:481:MET:HE1	1.75	0.51
1:B:221:THR:OG1	1:B:224:GLN:HG3	2.10	0.51
1:A:5:THR:HG23	1:A:8:GLN:OE1	2.10	0.51
1:A:157:ILE:HD12	1:A:211:PHE:CE1	2.45	0.51
1:A:636:PHE:HB2	1:A:640:GLY:O	2.11	0.51
1:B:436:LEU:O	1:B:442:VAL:HA	2.09	0.51
1:B:677:PHE:HD2	1:B:677:PHE:N	2.08	0.51
1:A:422:LYS:O	1:A:424:ASP:N	2.44	0.51
1:B:152:LYS:HG3	1:B:200:VAL:CG2	2.40	0.51
1:B:556:ILE:N	1:B:556:ILE:HD12	2.25	0.51
1:B:659:ILE:O	1:B:663:VAL:HG23	2.11	0.51
1:B:558:PRO:HG3	1:B:778:PHE:CZ	2.45	0.51
1:B:806:SER:O	1:B:808:PRO:HD3	2.10	0.51
1:B:576:LEU:HD22	1:B:842:LEU:HG	1.91	0.51
1:A:584:ASN:ND2	1:A:584:ASN:N	2.57	0.51
1:A:608:PRO:HG3	1:A:636:PHE:CD2	2.46	0.51
1:B:740:VAL:HG21	1:B:766:PHE:HZ	1.74	0.51
1:A:249:PHE:HB2	1:A:258:THR:HG23	1.92	0.50
1:A:414:GLN:OE1	1:A:477:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLU:HA	1:A:494:GLU:OE1	2.10	0.50
1:B:418:TYR:CG	1:B:419:VAL:N	2.79	0.50
1:B:500:ASP:CB	1:B:552:VAL:HG11	2.41	0.50
1:A:194:ASP:HB3	1:A:196:VAL:HG23	1.93	0.50
1:A:259:ASN:O	1:A:260:LYS:HE2	2.11	0.50
1:B:229:TYR:CE2	1:B:276:PHE:HB3	2.46	0.50
1:B:10:ARG:NH1	1:B:449:PRO:CD	2.74	0.50
1:A:429:LYS:HG2	1:A:462:PHE:CZ	2.46	0.50
1:A:584:ASN:HD21	1:A:694:HIS:HB2	1.76	0.50
1:B:454:ILE:HD13	1:B:455:GLY:O	2.11	0.50
1:A:601:ILE:HD13	1:A:606:ILE:HB	1.93	0.50
1:A:13:MET:CB	1:A:452:ASN:HD21	2.24	0.50
1:A:222:ILE:H	1:A:222:ILE:CD1	2.24	0.50
1:B:588:LEU:HD12	1:B:588:LEU:C	2.32	0.50
1:A:466:THR:OG1	1:A:480:VAL:HB	2.11	0.50
1:A:666:ALA:CB	1:A:709:MET:HB3	2.41	0.50
1:B:111:PHE:HB3	1:B:114:GLU:HB2	1.93	0.50
1:B:325:ARG:O	1:B:329:PRO:HG3	2.11	0.50
1:B:379:MET:SD	1:B:470:THR:HG22	2.52	0.50
1:B:710:ARG:HH11	1:B:710:ARG:HG3	1.76	0.50
1:A:155:VAL:CG1	1:A:156:VAL:N	2.74	0.50
1:A:263:ASP:CG	1:A:264:ALA:N	2.65	0.50
1:A:357:TYR:CZ	1:A:476:HIS:HB2	2.46	0.50
1:A:711:ARG:CZ	1:A:838:TYR:HA	2.41	0.50
1:A:711:ARG:HG3	1:A:711:ARG:HH11	1.77	0.50
1:A:17:THR:CG2	1:A:92:LYS:HG3	2.41	0.50
1:B:169:VAL:CG1	1:B:170:SER:N	2.74	0.50
1:B:228:ARG:HG2	1:B:232:LYS:NZ	2.25	0.50
1:B:414:GLN:OE1	1:B:477:ASN:ND2	2.45	0.50
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.94	0.49
1:A:181:THR:O	1:A:185:VAL:HG23	2.12	0.49
1:A:663:VAL:HG13	1:A:709:MET:HG2	1.94	0.49
1:B:288:ILE:HD12	1:B:296:ILE:HG22	1.93	0.49
1:B:718:LEU:HB3	1:B:835:TRP:HB3	1.94	0.49
1:B:261:ASP:OD1	1:B:262:THR:HG23	2.12	0.49
1:A:374:PRO:O	1:A:404:THR:HG22	2.12	0.49
1:A:578:LYS:HA	1:A:585:ARG:HG2	1.94	0.49
1:A:159:LYS:HE2	3:A:902:GDP:C4	2.48	0.49
1:A:570:GLU:HA	1:A:590:ALA:O	2.12	0.49
1:A:587:TYR:N	1:A:587:TYR:CD2	2.78	0.49
1:A:655:TYR:CB	1:A:658:GLU:HG3	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:TYR:HB3	1:B:658:GLU:HG3	1.95	0.49
1:A:104:ASP:OD1	1:A:106:PRO:CG	2.61	0.49
1:A:391:LYS:HD3	1:A:391:LYS:N	2.26	0.49
1:B:694:HIS:CB	1:B:700:ARG:HD3	2.41	0.49
1:B:740:VAL:CG2	1:B:766:PHE:CE1	2.92	0.49
1:B:270:GLU:HG2	1:B:275:MET:HE2	1.93	0.49
1:B:694:HIS:HB3	1:B:700:ARG:CG	2.43	0.49
1:B:655:TYR:HB2	1:B:700:ARG:HH22	1.77	0.49
1:A:206:ARG:NH2	1:A:242:ASP:OD1	2.44	0.49
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.93	0.49
1:B:6:VAL:CG1	1:B:445:ILE:HD12	2.42	0.49
1:B:391:LYS:O	1:B:393:ARG:HG2	2.12	0.48
1:B:740:VAL:HG12	1:B:744:TYR:CE2	2.35	0.48
1:A:16:VAL:HG23	1:A:346:VAL:CG2	2.43	0.48
1:B:448:CYS:SG	1:B:452:ASN:HB2	2.53	0.48
1:A:150:ARG:N	1:A:150:ARG:CD	2.75	0.48
1:A:434:VAL:C	1:A:445:ILE:HG22	2.34	0.48
1:A:457:VAL:O	1:A:457:VAL:CG2	2.61	0.48
1:A:584:ASN:N	1:A:584:ASN:HD22	2.10	0.48
1:B:157:ILE:HD12	1:B:211:PHE:CE1	2.48	0.48
1:B:722:PRO:O	1:B:723:LYS:HD2	2.13	0.48
1:A:691:VAL:HG12	1:A:693:LEU:HG	1.95	0.48
1:A:717:PHE:HD2	1:A:718:LEU:HD13	1.78	0.48
1:B:567:VAL:O	1:B:592:PRO:HB3	2.13	0.48
1:B:226:ALA:CB	1:B:241:MET:HB3	2.44	0.48
1:B:247:ASP:HA	1:B:249:PHE:HE1	1.79	0.48
1:B:501:LEU:HB3	1:B:502:PRO:HD3	1.96	0.48
1:B:576:LEU:HD22	1:B:842:LEU:CD1	2.44	0.48
1:A:411:VAL:HG12	1:A:412:ARG:N	2.28	0.48
1:A:488:VAL:O	1:A:781:THR:HG21	2.14	0.48
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.78	0.48
1:B:839:TYR:CE2	1:B:841:LYS:HA	2.49	0.48
1:A:183:GLU:O	1:A:187:VAL:HG23	2.14	0.48
1:B:139:THR:O	1:B:142:VAL:N	2.47	0.48
1:B:270:GLU:CG	1:B:275:MET:HG2	2.44	0.48
1:B:625:TRP:HH2	1:B:645:LEU:HD12	1.79	0.48
1:A:371:ASN:O	1:A:372:CYS:C	2.51	0.48
1:A:13:MET:CG	1:A:452:ASN:ND2	2.76	0.48
1:B:279:ASP:O	1:B:283:ARG:HG3	2.14	0.48
1:B:350:ALA:O	1:B:370:LYS:HE3	2.14	0.48
1:B:386:VAL:HG13	1:B:395:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG21	1:A:184:SER:HB2	1.96	0.47
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.76	0.47
1:A:70:ILE:HG22	1:A:388:THR:CG2	2.42	0.47
1:A:86:VAL:HG21	1:A:96:ASN:OD1	2.14	0.47
1:B:377:ASP:HA	1:B:471:THR:CG2	2.44	0.47
1:B:411:VAL:HG12	1:B:412:ARG:N	2.29	0.47
1:B:45:ILE:HD12	1:B:76:SER:HB3	1.95	0.47
1:B:576:LEU:HD21	1:B:585:ARG:NH1	2.29	0.47
1:B:659:ILE:HG22	1:B:705:ILE:HG13	1.95	0.47
1:A:653:VAL:CG1	1:A:656:LEU:HB2	2.44	0.47
1:B:318:ALA:O	1:B:322:VAL:HG23	2.14	0.47
1:B:545:LEU:HA	1:B:549:HIS:HB2	1.95	0.47
1:A:149:GLU:O	1:A:352:ARG:NH1	2.47	0.47
1:A:260:LYS:C	1:A:262:THR:H	2.16	0.47
1:A:378:LEU:O	1:A:470:THR:HA	2.15	0.47
1:A:100:ILE:HD13	1:A:338:ILE:HG21	1.96	0.47
1:A:228:ARG:C	1:A:230:ALA:H	2.18	0.47
1:A:218:TRP:HA	1:A:328:LEU:O	2.13	0.47
1:A:574:THR:HG21	1:A:587:TYR:HB3	1.97	0.47
1:A:615:ARG:HB2	1:A:615:ARG:NH1	2.29	0.47
1:B:305:ILE:HD11	1:B:327:PHE:CD1	2.50	0.47
1:B:70:ILE:CG2	1:B:388:THR:HG22	2.44	0.47
1:A:13:MET:HB3	1:A:452:ASN:ND2	2.29	0.47
1:B:100:ILE:HD12	1:B:338:ILE:CG2	2.45	0.47
1:B:459:ILE:HG22	1:B:459:ILE:O	2.14	0.47
1:A:759:GLN:HG3	1:A:760:ARG:H	1.77	0.47
1:B:563:TYR:O	1:B:679:GLU:CG	2.63	0.47
1:B:699:HIS:O	1:B:700:ARG:HG2	2.15	0.47
1:B:737:GLU:N	1:B:766:PHE:CE2	2.83	0.47
1:A:150:ARG:HD3	1:A:150:ARG:H	1.76	0.47
1:B:137:VAL:O	1:B:138:GLN:C	2.53	0.47
1:B:601:ILE:HD13	1:B:606:ILE:HB	1.97	0.47
1:A:810:ASP:O	1:A:812:THR:N	2.47	0.47
1:B:46:ILE:HG22	1:B:47:SER:N	2.30	0.47
1:A:233:PHE:O	1:A:235:VAL:HG23	2.14	0.46
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.97	0.46
1:A:637:GLY:O	1:A:644:ASN:HB2	2.14	0.46
1:A:760:ARG:CG	1:A:764:PRO:CG	2.92	0.46
1:B:145:GLN:HB2	1:B:145:GLN:HE21	1.54	0.46
1:B:633:ILE:HG22	1:B:647:ILE:HG13	1.96	0.46
1:B:698:ILE:HG23	1:B:699:HIS:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASP:C	1:A:151:ILE:HG23	2.36	0.46
1:B:470:THR:HG21	1:B:475:ALA:HB1	1.97	0.46
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.98	0.46
1:A:418:TYR:CE1	1:A:426:LEU:CG	2.98	0.46
1:B:228:ARG:C	1:B:230:ALA:H	2.19	0.46
1:B:232:LYS:O	1:B:233:PHE:HB3	2.16	0.46
1:B:433:ARG:HB3	1:B:457:VAL:CG1	2.45	0.46
1:A:81:MET:HG3	1:A:339:VAL:HG11	1.98	0.46
1:B:515:ASP:O	1:B:518:VAL:HG12	2.16	0.46
1:B:144:ARG:HE	1:B:188:ILE:HG23	1.80	0.46
1:A:157:ILE:HD12	1:A:211:PHE:HE1	1.81	0.46
1:A:24:VAL:HG21	1:A:36:THR:HG22	1.98	0.46
1:A:68:ILE:HD12	1:A:390:ASP:HB2	1.96	0.46
1:A:732:GLU:HB3	1:A:795:GLN:HE21	1.81	0.46
1:A:810:ASP:OD1	1:A:812:THR:HG23	2.14	0.46
1:A:196:VAL:C	1:A:197:LEU:HD12	2.35	0.46
1:B:21:ASN:HD22	1:B:101:ASN:HB2	1.81	0.46
1:B:150:ARG:CZ	1:B:196:VAL:HG11	2.46	0.46
1:B:434:VAL:CG1	1:B:454:ILE:HD11	2.46	0.46
1:B:377:ASP:CA	1:B:471:THR:HG22	2.46	0.46
1:B:785:ARG:HE	1:B:785:ARG:HB2	1.58	0.46
1:A:263:ASP:OD1	1:A:264:ALA:N	2.49	0.46
1:A:577:SER:HB2	1:A:712:ALA:HB2	1.98	0.46
1:A:764:PRO:O	1:A:765:LEU:CB	2.57	0.46
1:A:764:PRO:C	1:A:765:LEU:CG	2.60	0.46
1:B:103:ILE:N	1:B:103:ILE:HD12	2.30	0.46
1:B:316:GLY:O	1:B:317:LYS:C	2.54	0.46
1:A:13:MET:CB	1:A:452:ASN:ND2	2.79	0.46
1:A:607:ASN:HA	1:A:608:PRO:HD3	1.84	0.46
1:B:500:ASP:HB3	1:B:552:VAL:HG11	1.98	0.46
1:B:77:LEU:HB2	1:B:100:ILE:HB	1.98	0.46
1:B:718:LEU:HD23	1:B:835:TRP:HA	1.98	0.46
1:A:243:ARG:C	1:A:245:TRP:H	2.20	0.45
1:A:422:LYS:N	1:A:422:LYS:CD	2.78	0.45
1:A:413:ILE:CD1	1:A:459:ILE:HG23	2.46	0.45
1:A:785:ARG:HB2	1:A:785:ARG:HE	1.39	0.45
1:B:258:THR:OG1	1:B:259:ASN:N	2.49	0.45
1:B:39:LEU:HB3	1:B:77:LEU:HD21	1.97	0.45
1:B:795:GLN:HG3	1:B:795:GLN:O	2.17	0.45
1:A:374:PRO:O	1:A:404:THR:CG2	2.64	0.45
1:A:650:THR:OG1	1:A:656:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:HIS:CG	1:A:695:ALA:H	2.34	0.45
1:B:139:THR:O	1:B:140:GLU:C	2.55	0.45
1:B:696:ASP:OD1	1:B:697:ALA:N	2.49	0.45
1:B:836:GLN:H	1:B:836:GLN:HE21	1.59	0.45
1:A:103:ILE:HD12	1:A:397:PHE:HZ	1.82	0.45
1:A:162:ARG:NH1	1:A:166:GLU:OE1	2.50	0.45
1:A:489:VAL:CG1	1:A:781:THR:CG2	2.93	0.45
1:B:159:LYS:HG2	3:B:1902:GDP:C6	2.51	0.45
1:B:288:ILE:CD1	1:B:296:ILE:HG22	2.45	0.45
1:A:660:LYS:O	1:A:664:VAL:HG23	2.16	0.45
1:B:211:PHE:HD2	1:B:220:PHE:CE1	2.35	0.45
1:A:24:VAL:O	1:A:32:LYS:HE3	2.17	0.45
1:B:24:VAL:O	1:B:32:LYS:HE3	2.16	0.45
1:B:483:PHE:O	1:B:485:VAL:HG22	2.17	0.45
1:B:563:TYR:O	1:B:679:GLU:HG3	2.16	0.45
1:A:380:LEU:HD23	1:A:380:LEU:C	2.37	0.45
1:A:504:LEU:O	1:A:504:LEU:HD12	2.17	0.45
1:A:814:LYS:O	1:A:818:ILE:HG12	2.17	0.45
1:B:806:SER:HB2	1:B:815:ALA:HB2	1.99	0.45
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.98	0.45
1:A:237:LYS:O	1:A:238:ALA:C	2.54	0.45
1:A:709:MET:O	1:A:710:ARG:C	2.55	0.45
1:B:345:PRO:HA	1:B:399:ARG:NH2	2.31	0.45
1:A:737:GLU:HB3	1:A:766:PHE:CE2	2.51	0.45
1:B:817:GLU:O	1:B:820:LEU:HB3	2.17	0.45
1:A:356:LEU:HD13	1:A:401:PHE:CE1	2.52	0.45
1:A:705:ILE:O	1:A:706:ILE:C	2.55	0.45
1:B:236:ASP:OD2	1:B:239:LYS:HB3	2.17	0.45
1:B:357:TYR:OH	1:B:476:HIS:HB2	2.17	0.45
1:B:579:SER:C	1:B:581:ASN:H	2.20	0.45
1:A:288:ILE:HD12	1:A:319:LEU:HD23	1.97	0.45
1:A:305:ILE:HD11	1:A:327:PHE:CD1	2.51	0.45
1:B:576:LEU:HD13	1:B:587:TYR:CE1	2.52	0.45
1:B:648:ASP:OD1	1:B:656:LEU:HD21	2.16	0.45
1:B:23:SER:HA	1:B:102:LEU:HD12	1.98	0.44
1:B:177:THR:HA	1:B:180:ARG:HE	1.83	0.44
1:B:625:TRP:CH2	1:B:645:LEU:HD12	2.53	0.44
1:A:284:LEU:O	1:A:288:ILE:HG12	2.17	0.44
1:A:393:ARG:CZ	1:A:460:ASP:CG	2.86	0.44
1:A:726:GLU:OE2	1:A:804:LEU:HD21	2.17	0.44
1:B:75:ILE:HD12	1:B:102:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:HG12	1:B:209:VAL:HG23	1.98	0.44
1:B:220:PHE:HA	1:B:224:GLN:OE1	2.17	0.44
1:B:552:VAL:HG13	1:B:553:PRO:CD	2.47	0.44
1:B:579:SER:HB2	1:B:580:PRO:CD	2.47	0.44
1:B:591:GLU:HB2	1:B:592:PRO:HD2	1.98	0.44
1:B:178:PHE:O	1:B:182:VAL:HG23	2.16	0.44
1:B:723:LYS:HA	1:B:808:PRO:CG	2.46	0.44
1:A:169:VAL:HG12	1:A:170:SER:O	2.18	0.44
1:A:694:HIS:CD2	1:A:696:ASP:H	2.35	0.44
1:A:764:PRO:CD	1:A:765:LEU:N	2.70	0.44
1:A:754:VAL:HA	1:A:770:ALA:CB	2.46	0.44
1:A:105:SER:N	1:A:106:PRO:HD3	2.31	0.44
1:B:411:VAL:HG12	1:B:412:ARG:H	1.82	0.44
1:A:321:LYS:O	1:A:325:ARG:HG3	2.17	0.44
1:A:367:ILE:O	1:A:370:LYS:HB2	2.17	0.44
1:B:46:ILE:HG22	1:B:47:SER:H	1.82	0.44
1:A:197:LEU:HD12	1:A:197:LEU:N	2.33	0.44
1:A:36:THR:O	1:A:40:VAL:HG23	2.18	0.44
1:A:46:ILE:CG2	1:A:47:SER:N	2.79	0.44
1:A:706:ILE:CB	1:A:707:PRO:HD3	2.35	0.44
1:B:378:LEU:HB3	1:B:471:THR:HB	1.98	0.44
1:B:581:ASN:C	1:B:583:HIS:H	2.21	0.44
1:A:544:ASP:O	1:A:548:ASP:HB2	2.17	0.44
1:B:167:LEU:N	1:B:167:LEU:HD12	2.33	0.44
1:A:829:LYS:HG3	1:A:831:GLU:H	1.83	0.44
1:B:378:LEU:H	1:B:471:THR:CG2	2.31	0.44
1:B:587:TYR:O	1:B:689:LEU:HB2	2.18	0.44
1:B:724:ILE:HD11	1:B:804:LEU:HD12	2.00	0.44
1:A:677:PHE:HD1	1:A:822:ALA:HB3	1.83	0.43
1:B:212:GLY:HA3	1:B:219:ALA:HA	2.00	0.43
1:A:104:ASP:OD1	1:A:106:PRO:HD3	2.18	0.43
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.54	0.43
1:B:415:GLY:HA3	1:B:425:ASP:OD1	2.17	0.43
1:B:615:ARG:NH1	1:B:615:ARG:CB	2.80	0.43
1:A:167:LEU:HD12	1:A:167:LEU:N	2.33	0.43
1:A:113:SER:O	1:A:481:MET:HE2	2.18	0.43
1:A:655:TYR:HD1	1:A:658:GLU:CD	2.21	0.43
1:B:27:HIS:CD2	1:B:28:VAL:O	2.69	0.43
1:B:500:ASP:HB3	1:B:552:VAL:HG21	2.00	0.43
1:B:751:ARG:NE	1:B:814:LYS:NZ	2.66	0.43
1:B:434:VAL:HG13	1:B:454:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLU:CB	1:B:267:LYS:HE3	2.49	0.43
1:B:70:ILE:HG22	1:B:388:THR:CB	2.49	0.43
1:B:564:ARG:HB2	1:B:725:GLN:HB2	2.00	0.43
1:B:6:VAL:HG13	1:B:445:ILE:HD12	2.00	0.43
1:B:157:ILE:HD12	1:B:211:PHE:HE1	1.83	0.43
1:A:669:TRP:CD1	1:A:710:ARG:NH1	2.86	0.43
1:A:764:PRO:O	1:A:765:LEU:CD2	2.57	0.43
1:B:174:LEU:HG	1:B:178:PHE:CE2	2.53	0.43
1:B:352:ARG:HG2	1:B:352:ARG:HH11	1.84	0.43
1:B:836:GLN:H	1:B:836:GLN:CD	2.22	0.43
1:A:390:ASP:O	1:A:393:ARG:HG2	2.18	0.43
1:B:156:VAL:HA	1:B:210:ALA:O	2.19	0.43
1:A:202:VAL:CG1	1:A:209:VAL:CG2	2.97	0.43
1:A:377:ASP:HB3	1:A:471:THR:HG22	2.00	0.43
1:A:378:LEU:H	1:A:471:THR:CG2	2.32	0.43
1:B:199:ASP:OD1	1:B:201:GLN:HG3	2.19	0.43
1:B:453:ILE:HA	1:B:453:ILE:HD13	1.85	0.43
1:B:569:SER:O	1:B:720:ALA:HB1	2.18	0.43
1:B:754:VAL:HG12	1:B:755:VAL:N	2.34	0.43
1:B:788:THR:O	1:B:791:GLN:HB2	2.18	0.43
1:A:434:VAL:HG12	1:A:445:ILE:HG21	2.01	0.43
1:B:120:ARG:NH1	1:B:481:MET:CE	2.82	0.43
1:B:650:THR:HG23	1:B:688:ILE:HG22	2.01	0.43
1:A:142:VAL:HA	1:A:145:GLN:OE1	2.19	0.42
1:A:202:VAL:CG1	1:A:209:VAL:HG22	2.49	0.42
1:A:156:VAL:HG22	1:A:210:ALA:HB3	2.00	0.42
1:B:374:PRO:O	1:B:403:GLY:HA2	2.19	0.42
1:B:123:ASP:CG	1:B:399:ARG:HH12	2.22	0.42
1:B:418:TYR:HB2	1:B:425:ASP:HB2	2.00	0.42
1:A:391:LYS:O	1:A:393:ARG:HG2	2.18	0.42
1:A:666:ALA:HB2	1:A:706:ILE:HA	2.00	0.42
1:A:723:LYS:HA	1:A:808:PRO:HG2	2.02	0.42
1:B:520:THR:HA	1:B:529:ILE:O	2.19	0.42
1:B:781:THR:HG23	1:B:782:GLY:N	2.34	0.42
1:A:589:LYS:HG3	1:A:689:LEU:HD11	2.02	0.42
1:B:10:ARG:HH12	1:B:449:PRO:CD	2.32	0.42
1:B:22:MET:HA	1:B:122:THR:HB	2.01	0.42
1:A:127:VAL:HG21	1:A:143:LEU:HD13	2.01	0.42
1:A:90:LYS:HG3	1:A:90:LYS:O	2.20	0.42
1:B:382:VAL:O	1:B:466:THR:HA	2.19	0.42
1:B:428:ILE:N	1:B:428:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:796:MET:SD	1:B:796:MET:N	2.93	0.42
1:A:591:GLU:HB2	1:A:592:PRO:HD2	2.01	0.42
1:A:86:VAL:O	1:A:86:VAL:HG12	2.18	0.42
1:B:615:ARG:HG2	1:B:619:MET:HE2	2.02	0.42
1:A:286:THR:O	1:A:290:ASN:HB2	2.19	0.42
1:A:556:ILE:CD1	1:A:556:ILE:N	2.83	0.42
1:B:400:VAL:HG12	1:B:450:ALA:HA	2.01	0.42
1:B:576:LEU:HD13	1:B:587:TYR:CD1	2.55	0.42
1:A:197:LEU:N	1:A:197:LEU:CD1	2.82	0.42
1:A:215:LEU:HB2	3:A:902:GDP:C5	2.55	0.42
1:A:391:LYS:C	1:A:393:ARG:H	2.23	0.42
1:A:681:MET:CE	1:A:717:PHE:CD1	3.03	0.42
1:A:711:ARG:HH12	1:A:838:TYR:HA	1.77	0.42
1:B:348:ALA:HA	1:B:351:TYR:CZ	2.55	0.42
1:B:390:ASP:HB3	1:B:393:ARG:HB2	2.01	0.42
1:B:293:LYS:O	1:B:296:ILE:HG12	2.20	0.42
1:B:377:ASP:HA	1:B:471:THR:HG22	2.02	0.42
1:B:522:MET:HE1	1:B:528:HIS:CE1	2.55	0.42
1:B:567:VAL:HG13	1:B:717:PHE:CE1	2.55	0.42
1:B:809:LEU:N	1:B:809:LEU:HD12	2.35	0.42
1:A:178:PHE:O	1:A:182:VAL:HG23	2.20	0.42
1:A:274:ASN:HA	1:A:278:LEU:HB2	2.01	0.42
1:A:432:GLN:HB3	1:A:457:VAL:O	2.19	0.42
1:A:562:ALA:O	1:A:727:PRO:HD3	2.19	0.42
1:B:311:GLU:HA	1:B:314:LEU:CG	2.47	0.42
1:B:671:THR:HA	1:B:681:MET:HG3	2.02	0.42
1:B:693:LEU:HD13	1:B:700:ARG:NH1	2.35	0.42
1:B:806:SER:HB2	1:B:815:ALA:CB	2.50	0.42
1:A:730:LEU:HB2	1:A:799:ASP:HB2	2.01	0.41
1:B:231:LYS:C	1:B:233:PHE:N	2.64	0.41
1:B:357:TYR:CZ	1:B:476:HIS:HB2	2.55	0.41
1:B:357:TYR:CE2	1:B:359:GLY:HA3	2.55	0.41
1:B:397:PHE:HD1	1:B:437:MET:HG3	1.85	0.41
1:B:724:ILE:O	1:B:724:ILE:HD13	2.20	0.41
1:A:435:VAL:HG12	1:A:444:PRO:HA	2.02	0.41
1:A:760:ARG:HE	1:A:761:PRO:HD2	1.83	0.41
1:B:204:PRO:HG3	1:B:209:VAL:HG21	2.01	0.41
1:B:270:GLU:HG2	1:B:275:MET:HG2	2.02	0.41
1:B:136:CYS:O	1:B:139:THR:HB	2.20	0.41
1:B:391:LYS:HA	1:B:391:LYS:HD3	1.76	0.41
1:B:593:ILE:HG12	1:B:685:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:TRP:HZ3	1:B:660:LYS:HA	1.77	0.41
1:A:249:PHE:N	1:A:249:PHE:CD2	2.88	0.41
1:A:625:TRP:HH2	1:A:645:LEU:HD12	1.86	0.41
1:A:760:ARG:HG2	1:A:764:PRO:HD2	2.02	0.41
1:B:662:SER:OG	1:B:702:GLY:HA2	2.20	0.41
1:B:562:ALA:O	1:B:727:PRO:HD3	2.20	0.41
1:A:760:ARG:CZ	1:A:761:PRO:HD2	2.51	0.41
1:B:86:VAL:CG1	1:B:93:THR:HG21	2.50	0.41
1:A:152:LYS:HG3	1:A:200:VAL:HG23	2.02	0.41
1:A:413:ILE:HB	1:A:427:PHE:HB2	2.01	0.41
1:A:700:ARG:O	1:A:705:ILE:HG12	2.21	0.41
1:A:702:GLY:O	1:A:706:ILE:HD13	2.20	0.41
1:B:202:VAL:HG13	1:B:208:THR:HB	2.01	0.41
1:B:352:ARG:NH1	1:B:356:LEU:HD21	2.34	0.41
1:B:434:VAL:HG13	1:B:454:ILE:HD11	2.00	0.41
1:B:677:PHE:HD2	1:B:677:PHE:H	1.67	0.41
1:B:81:MET:HA	1:B:81:MET:CE	2.50	0.41
1:A:17:THR:HG21	1:A:92:LYS:CG	2.47	0.41
1:A:593:ILE:HG22	1:A:594:ASP:N	2.35	0.41
1:B:243:ARG:O	1:B:272:ALA:HB3	2.20	0.41
1:B:406:LYS:O	1:B:409:GLN:HB3	2.21	0.41
1:B:78:TYR:OH	1:B:80:GLU:HG3	2.21	0.41
1:B:81:MET:O	1:B:96:ASN:HB3	2.21	0.41
1:A:298:VAL:HG12	1:A:302:LYS:HE3	2.02	0.41
1:A:361:ALA:HA	1:A:366:CYS:SG	2.61	0.41
1:A:93:THR:HG22	1:A:94:ASP:N	2.36	0.41
1:B:267:LYS:HA	1:B:268:PRO:HD3	1.96	0.41
1:B:275:MET:HA	1:B:275:MET:HE2	2.02	0.41
1:B:739:ALA:C	1:B:741:GLY:N	2.74	0.41
1:B:110:ASP:C	1:B:789:GLY:HA3	2.40	0.41
1:B:751:ARG:CD	1:B:814:LYS:HZ3	2.33	0.41
1:A:35:LEU:O	1:A:38:SER:HB3	2.21	0.41
1:A:607:ASN:O	1:A:615:ARG:HD3	2.21	0.41
1:A:633:ILE:HG13	1:A:633:ILE:O	2.20	0.41
1:B:607:ASN:HA	1:B:608:PRO:HD3	1.87	0.41
1:B:710:ARG:NH1	1:B:710:ARG:HG3	2.35	0.41
1:A:377:ASP:HA	1:A:471:THR:CG2	2.50	0.41
1:A:482:LYS:HA	1:A:482:LYS:HD3	1.87	0.41
1:A:22:MET:HA	1:A:122:THR:HB	2.02	0.41
1:A:356:LEU:HB3	1:A:478:MET:CE	2.50	0.41
1:A:694:HIS:H	1:A:700:ARG:CD	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ARG:NH2	1:A:842:LEU:C	2.68	0.41
1:A:391:LYS:O	1:A:393:ARG:N	2.54	0.40
1:A:411:VAL:HG12	1:A:412:ARG:H	1.86	0.40
1:B:251:ASN:ND2	1:B:269:LEU:HD21	2.37	0.40
1:B:81:MET:HG3	1:B:339:VAL:HG11	2.03	0.40
1:B:118:ALA:O	1:B:121:VAL:HG22	2.21	0.40
1:B:523:SER:HB3	1:B:529:ILE:CD1	2.51	0.40
1:A:690:ASP:OD1	1:A:691:VAL:N	2.54	0.40
1:B:194:ASP:CB	1:B:196:VAL:HG12	2.49	0.40
1:B:153:PRO:HD2	1:B:200:VAL:HG22	2.03	0.40
1:B:279:ASP:HB3	1:B:280:PRO:CD	2.42	0.40
1:B:500:ASP:O	1:B:501:LEU:C	2.59	0.40
1:A:28:VAL:HG23	1:A:138:GLN:OE1	2.21	0.40
1:A:169:VAL:HG12	1:A:170:SER:N	2.36	0.40
1:A:425:ASP:C	1:A:426:LEU:O	2.59	0.40
1:A:565:GLU:O	1:A:681:MET:HA	2.20	0.40
1:B:237:LYS:O	1:B:241:MET:HG2	2.20	0.40
1:B:254:THR:O	1:B:256:LYS:HG3	2.21	0.40
1:B:75:ILE:H	1:B:75:ILE:HD12	1.85	0.40
1:B:172:GLU:HA	1:B:274:ASN:ND2	2.29	0.40
1:B:288:ILE:HD12	1:B:288:ILE:N	2.35	0.40
1:B:368:ALA:O	1:B:372:CYS:N	2.54	0.40
1:B:515:ASP:HA	1:B:516:PRO:HD3	1.95	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	818/842 (97%)	729 (89%)	67 (8%)	22 (3%)	5	19
1	B	805/842 (96%)	692 (86%)	95 (12%)	18 (2%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1623/1684 (96%)	1421 (88%)	162 (10%)	40 (2%)	5	21

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	PHE
1	A	424	ASP
1	A	765	LEU
1	B	112	SER
1	B	233	PHE
1	B	235	VAL
1	B	765	LEU
1	A	108	HIS
1	A	234	GLY
1	A	392	GLY
1	A	418	TYR
1	B	418	TYR
1	B	420	PRO
1	B	479	LYS
1	B	654	GLN
1	B	698	ILE
1	B	806	SER
1	A	244	LEU
1	A	426	LEU
1	A	465	LYS
1	A	479	LYS
1	A	498	ALA
1	A	654	GLN
1	A	737	GLU
1	A	811	PRO
1	B	317	LYS
1	A	677	PHE
1	B	166	GLU
1	B	811	PRO
1	A	261	ASP
1	A	292	LYS
1	B	113	SER
1	B	329	PRO
1	B	450	ALA
1	B	460	ASP
1	A	329	PRO
1	B	83	ASP

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Mol	Chain	Res	Type
1	A	701	GLY
1	A	134	GLY
1	A	580	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/715 (98%)	661 (95%)	38 (5%)	22	54
1	B	692/715 (97%)	650 (94%)	42 (6%)	18	48
All	All	1391/1430 (97%)	1311 (94%)	80 (6%)	20	50

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	102	LEU
1	A	150	ARG
1	A	154	VAL
1	A	183	GLU
1	A	194	ASP
1	A	196	VAL
1	A	206	ARG
1	A	236	ASP
1	A	261	ASP
1	A	308	LYS
1	A	404	THR
1	A	424	ASP
1	A	457	VAL
1	A	460	ASP
1	A	471	THR
1	A	476	HIS
1	A	483	PHE
1	A	533	THR
1	A	540	ILE

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Mol	Chain	Res	Type
1	A	544	ASP
1	A	548	ASP
1	A	585	ARG
1	A	587	TYR
1	A	594	ASP
1	A	599	LEU
1	A	661	ASP
1	A	677	PHE
1	A	696	ASP
1	A	708	THR
1	A	718	LEU
1	A	723	LYS
1	A	735	CYS
1	A	759	GLN
1	A	785	ARG
1	A	796	MET
1	A	806	SER
1	A	829	LYS
1	B	36	THR
1	B	75	ILE
1	B	110	ASP
1	B	145	GLN
1	B	154	VAL
1	B	168	GLN
1	B	183	GLU
1	B	192	TYR
1	B	194	ASP
1	B	225	PHE
1	B	249	PHE
1	B	362	ASP
1	B	386	VAL
1	B	404	THR
1	B	410	LYS
1	B	420	PRO
1	B	447	ASP
1	B	454	ILE
1	B	460	ASP
1	B	461	GLN
1	B	471	THR
1	B	476	HIS
1	B	482	LYS
1	B	485	VAL

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Mol	Chain	Res	Type
1	B	501	LEU
1	B	533	THR
1	B	540	ILE
1	B	543	GLN
1	B	548	ASP
1	B	596	GLU
1	B	599	LEU
1	B	626	ASP
1	B	677	PHE
1	B	708	THR
1	B	718	LEU
1	B	723	LYS
1	B	724	ILE
1	B	731	VAL
1	B	796	MET
1	B	814	LYS
1	B	831	GLU
1	B	836	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	A	452	ASN
1	A	477	ASN
1	A	583	HIS
1	A	584	ASN
1	A	694	HIS
1	A	753	GLN
1	A	795	GLN
1	A	800	HIS
1	B	21	ASN
1	B	101	ASN
1	B	145	GLN
1	B	168	GLN
1	B	201	GLN
1	B	349	GLN
1	B	476	HIS
1	B	477	ASN
1	B	528	HIS
1	B	549	HIS
1	B	699	HIS

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Mol	Chain	Res	Type
1	B	734	GLN
1	B	738	GLN
1	B	748	ASN
1	B	791	GLN
1	B	836	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GDP	A	902	-	24,30,30	1.49	4 (16%)	31,47,47	1.88	5 (16%)
3	GDP	B	1902	-	24,30,30	1.49	4 (16%)	31,47,47	1.96	5 (16%)
2	MOU	B	1901	-	45,54,54	2.40	12 (26%)	37,85,85	1.49	4 (10%)
2	MOU	A	901	-	45,54,54	2.43	10 (22%)	37,85,85	1.52	4 (10%)

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	GDP	A	902	-	-	3/12/32/32	0/3/3/3
3	GDP	B	1902	-	-	2/12/32/32	0/3/3/3
2	MOU	B	1901	-	-	5/23/132/132	0/8/6/6
2	MOU	A	901	-	-	3/23/132/132	0/8/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1901	MOU	C9-C23	7.61	1.63	1.50
2	A	901	MOU	C9-C23	7.40	1.62	1.50
2	A	901	MOU	C5-C4	6.99	1.43	1.32
2	B	1901	MOU	C5-C4	6.57	1.42	1.32
2	A	901	MOU	C13-C10	5.78	1.63	1.54
2	B	1901	MOU	C13-C10	5.45	1.62	1.54
2	B	1901	MOU	C6-C5	4.73	1.57	1.50
3	A	902	GDP	C6-N1	4.66	1.41	1.33
3	B	1902	GDP	C6-N1	4.62	1.41	1.33
2	B	1901	MOU	C9-C8	4.44	1.71	1.58
2	A	901	MOU	C13-C15	4.33	1.59	1.53
2	A	901	MOU	C9-C8	4.10	1.70	1.58
2	A	901	MOU	C6-C5	3.89	1.56	1.50
2	B	1901	MOU	O29-C28	3.77	1.51	1.41
2	A	901	MOU	C7-C6	3.67	1.58	1.53
2	A	901	MOU	O27-C28	3.58	1.46	1.40
2	B	1901	MOU	C7-C6	3.49	1.58	1.53
2	A	901	MOU	C7-C8	3.49	1.60	1.55
2	B	1901	MOU	C13-C15	3.28	1.58	1.53
3	A	902	GDP	C2-N1	3.21	1.41	1.35
2	A	901	MOU	O29-C28	3.16	1.49	1.41
2	B	1901	MOU	C7-C8	2.97	1.59	1.55
3	B	1902	GDP	C2-N1	2.95	1.40	1.35
2	B	1901	MOU	C26-C10	2.88	1.58	1.53
2	B	1901	MOU	O27-C28	2.76	1.44	1.40
3	B	1902	GDP	C4-N3	2.53	1.39	1.35
3	A	902	GDP	O4'-C1'	2.12	1.44	1.41
3	B	1902	GDP	O4'-C1'	2.12	1.44	1.41
2	B	1901	MOU	C15-C14	2.11	1.60	1.54
3	A	902	GDP	C4-N3	2.05	1.38	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1902	GDP	C5-C6-N1	-6.39	114.69	123.43
3	A	902	GDP	C5-C6-N1	-6.27	114.85	123.43
3	B	1902	GDP	C6-N1-C2	5.37	124.46	115.93
2	A	901	MOU	C7-C6-C10	5.15	113.58	103.54
2	B	1901	MOU	C7-C6-C10	5.12	113.52	103.54
3	A	902	GDP	C6-N1-C2	5.00	123.87	115.93
3	B	1902	GDP	N3-C2-N1	-4.43	121.31	127.22
3	A	902	GDP	N3-C2-N1	-4.08	121.78	127.22
2	A	901	MOU	C18-C14-C15	-3.98	97.93	103.64
2	B	1901	MOU	C18-C14-C15	-3.68	98.37	103.64
2	B	1901	MOU	O3-C-O	3.13	107.74	104.89
3	A	902	GDP	C6-C5-C4	-3.03	117.90	120.80
3	B	1902	GDP	C6-C5-C4	-3.01	117.92	120.80
2	A	901	MOU	C40-C39-C38	-2.98	103.08	113.62
2	A	901	MOU	O3-C-O	2.87	107.50	104.89
2	B	1901	MOU	C40-C39-C38	-2.66	104.22	113.62
3	B	1902	GDP	N2-C2-N3	2.52	121.90	117.79
3	A	902	GDP	N2-C2-N3	2.16	121.30	117.79

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	GDP	PA-O3A-PB-O2B
3	A	902	GDP	PA-O3A-PB-O3B
2	B	1901	MOU	C42-C43-C44-C45
2	A	901	MOU	C42-C43-C44-C45
2	A	901	MOU	C41-C42-C43-C44
2	B	1901	MOU	C41-C42-C43-C44
2	B	1901	MOU	O12-C11-C8-C7
3	B	1902	GDP	PA-O3A-PB-O3B
2	B	1901	MOU	O12-C11-C8-C14
2	A	901	MOU	O12-C11-C8-C14
2	B	1901	MOU	O12-C11-C8-C9
3	B	1902	GDP	PA-O3A-PB-O2B
3	A	902	GDP	PA-O3A-PB-O1B

There are no ring outliers.

4 monomers are involved in 8 short contacts:

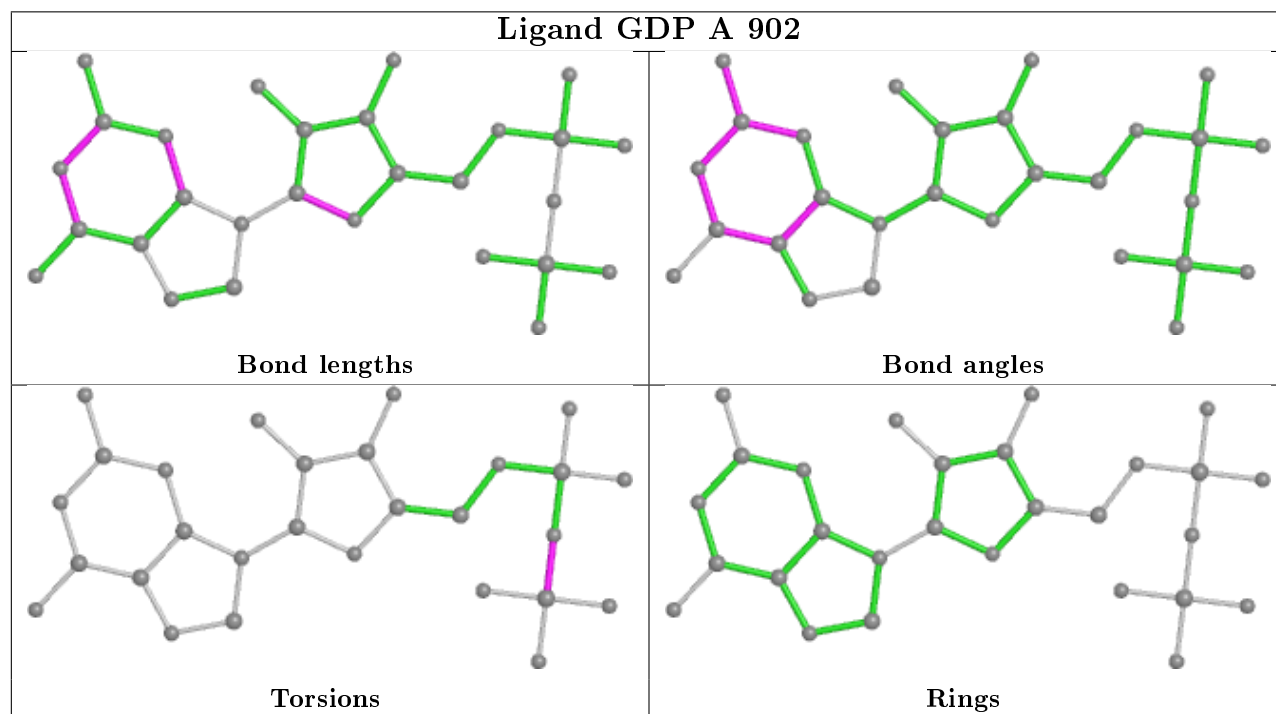
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GDP	4	0

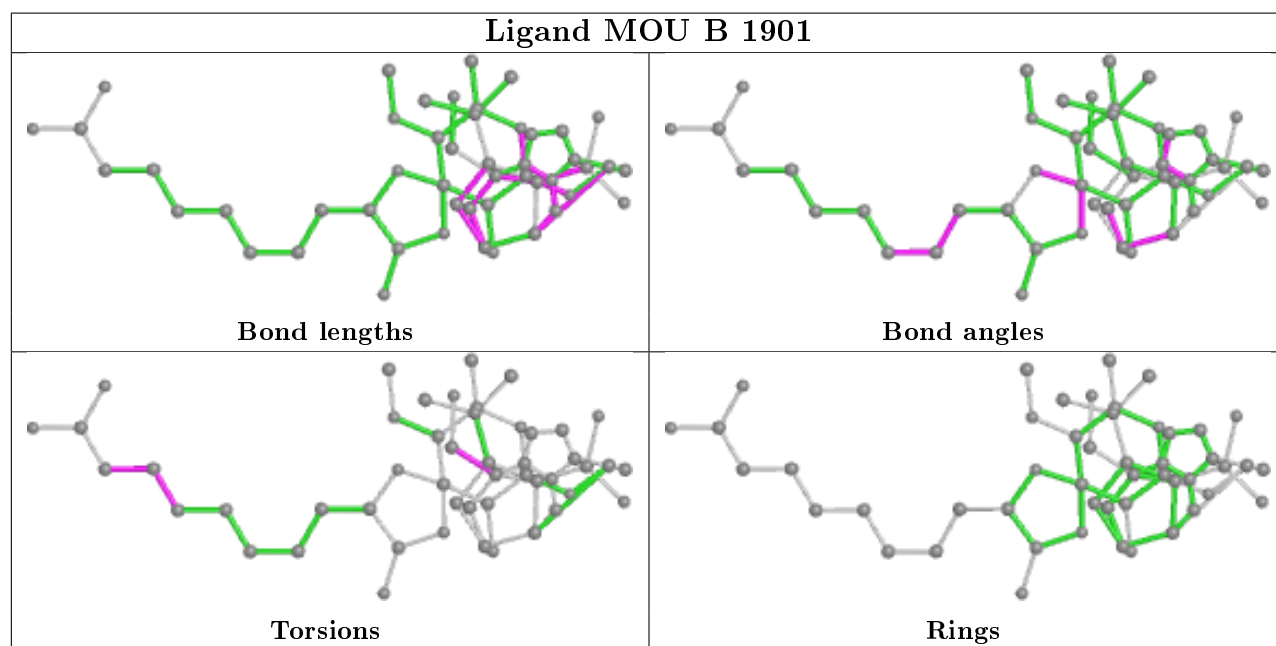
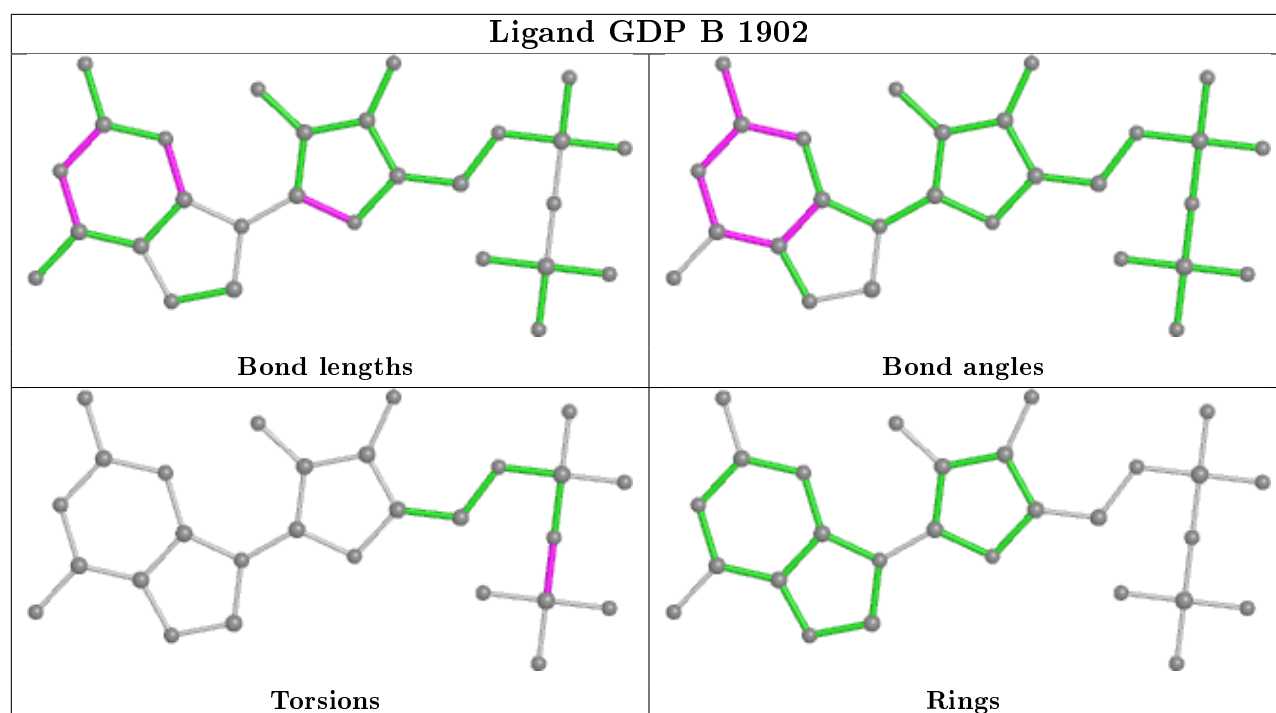
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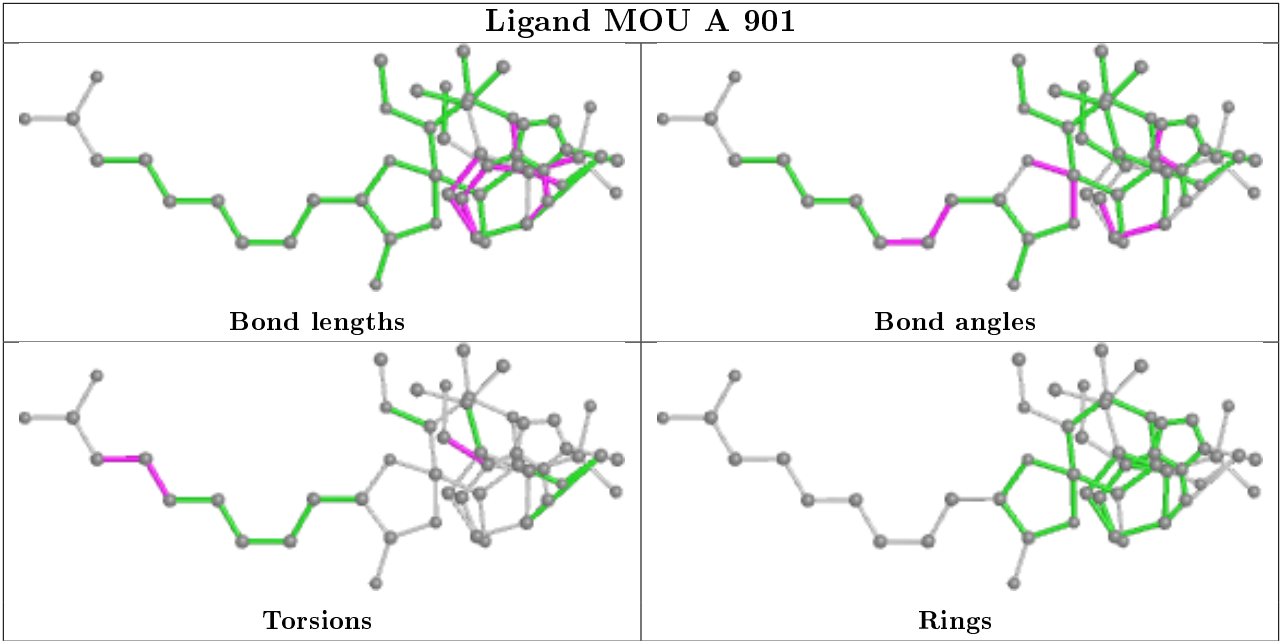
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1902	GDP	2	0
2	B	1901	MOU	1	0
2	A	901	MOU	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	764:PRO	C	765:LEU	N	1.14

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, 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	822/842 (97%)	0.04	29 (3%)	44 38	25, 62, 106, 133	0
1	B	813/842 (96%)	0.34	59 (7%)	15 11	37, 90, 125, 148	0
All	All	1635/1684 (97%)	0.19	88 (5%)	25 22	25, 76, 119, 148	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	GLY	7.0
1	B	113	SER	6.8
1	B	268	PRO	6.3
1	B	110	ASP	6.1
1	B	264	ALA	5.8
1	A	106	PRO	5.6
1	B	252	PRO	5.5
1	B	842	LEU	5.0
1	B	112	SER	5.0
1	B	254	THR	4.8
1	A	108	HIS	4.7
1	B	765	LEU	4.6
1	B	758	GLU	4.5
1	B	267	LYS	4.4
1	B	583	HIS	4.2
1	B	263	ASP	4.2
1	B	421	GLY	4.1
1	A	109	VAL	4.0
1	A	762	GLY	4.0
1	B	269	LEU	3.9
1	B	243	ARG	3.7
1	B	422	LYS	3.6
1	B	759	GLN	3.5
1	B	251	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	582	LYS	3.3
1	B	265	GLU	3.2
1	B	167	LEU	3.2
1	A	761	PRO	3.1
1	A	482	LYS	3.1
1	A	268	PRO	3.0
1	A	483	PHE	3.0
1	B	290	ASN	3.0
1	B	375	LYS	3.0
1	B	294	ASP	2.9
1	A	425	ASP	2.9
1	B	226	ALA	2.9
1	B	262	THR	2.9
1	B	764	PRO	2.9
1	B	700	ARG	2.8
1	B	86	VAL	2.8
1	B	232	LYS	2.8
1	A	392	GLY	2.8
1	B	253	LYS	2.8
1	B	256	LYS	2.7
1	B	737	GLU	2.7
1	A	110	ASP	2.7
1	B	234	GLY	2.7
1	A	763	THR	2.7
1	A	426	LEU	2.7
1	B	585	ARG	2.6
1	A	693	LEU	2.6
1	A	263	ASP	2.6
1	A	585	ARG	2.6
1	B	6	VAL	2.6
1	A	266	GLY	2.6
1	B	698	ILE	2.6
1	B	766	PHE	2.6
1	B	307	LEU	2.5
1	A	584	ASN	2.5
1	A	264	ALA	2.5
1	B	270	GLU	2.5
1	A	842	LEU	2.4
1	B	292	LYS	2.4
1	A	253	LYS	2.3
1	A	262	THR	2.3
1	B	655	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	583	HIS	2.3
1	A	424	ASP	2.3
1	B	398	GLY	2.3
1	B	230	ALA	2.3
1	B	293	LYS	2.3
1	A	210	ALA	2.2
1	B	694	HIS	2.2
1	B	298	VAL	2.2
1	A	582	LYS	2.2
1	B	260	LYS	2.1
1	B	355	GLN	2.1
1	B	739	ALA	2.1
1	B	295	GLU	2.1
1	B	576	LEU	2.1
1	B	195	GLU	2.1
1	A	421	GLY	2.0
1	B	132	ILE	2.0
1	A	361	ALA	2.0
1	B	381	TYR	2.0
1	B	400	VAL	2.0
1	A	423	LYS	2.0
1	B	255	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GDP	B	1902	28/28	0.92	0.16	106,107,109,109	0

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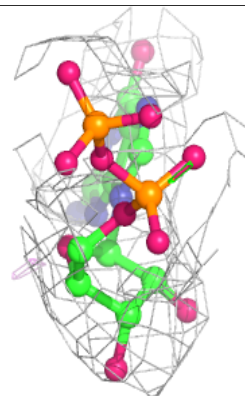
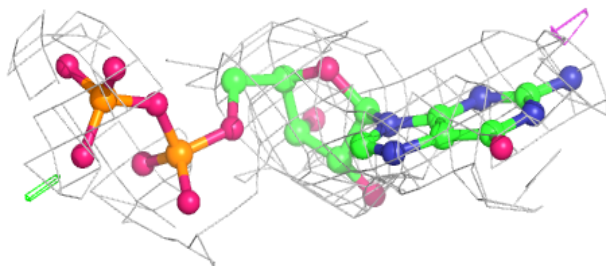
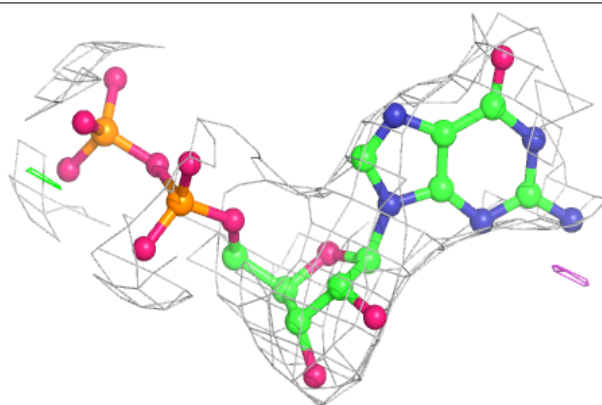
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MOU	B	1901	49/49	0.94	0.19	51,55,62,66	0
2	MOU	A	901	49/49	0.96	0.20	29,39,59,65	0
3	GDP	A	902	28/28	0.97	0.13	48,54,60,61	0

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.

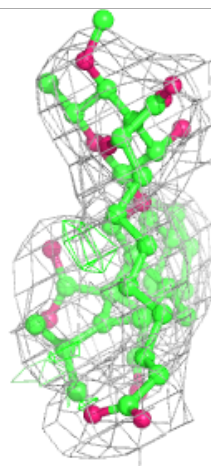
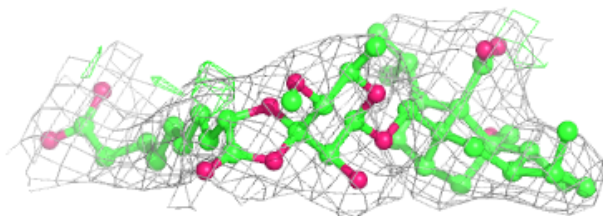
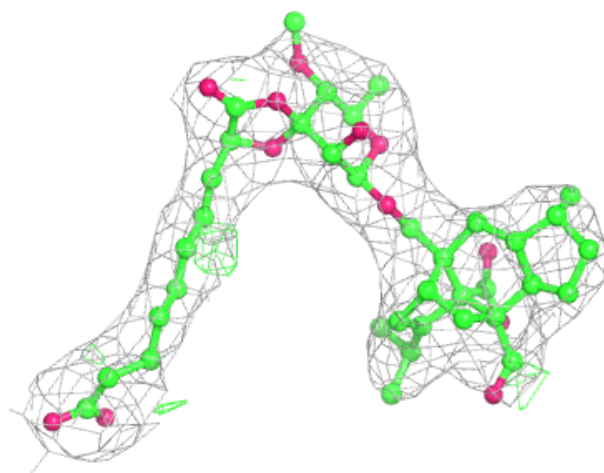
Electron density around GDP B 1902:

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



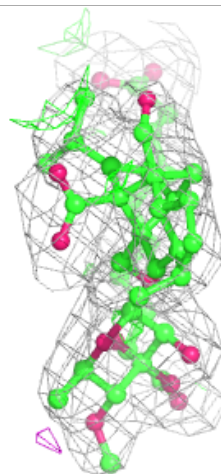
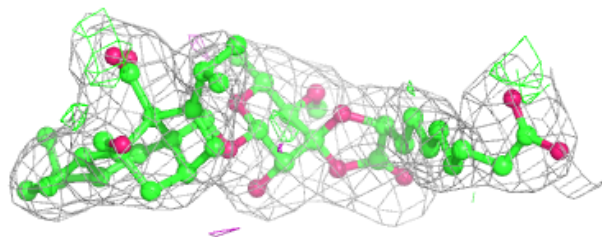
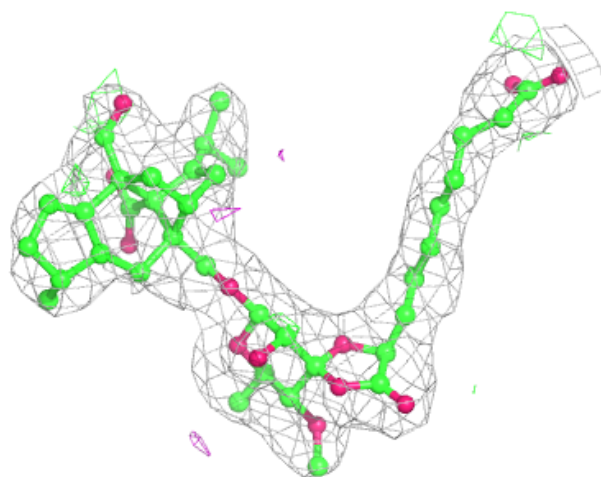
Electron density around MOU B 1901:

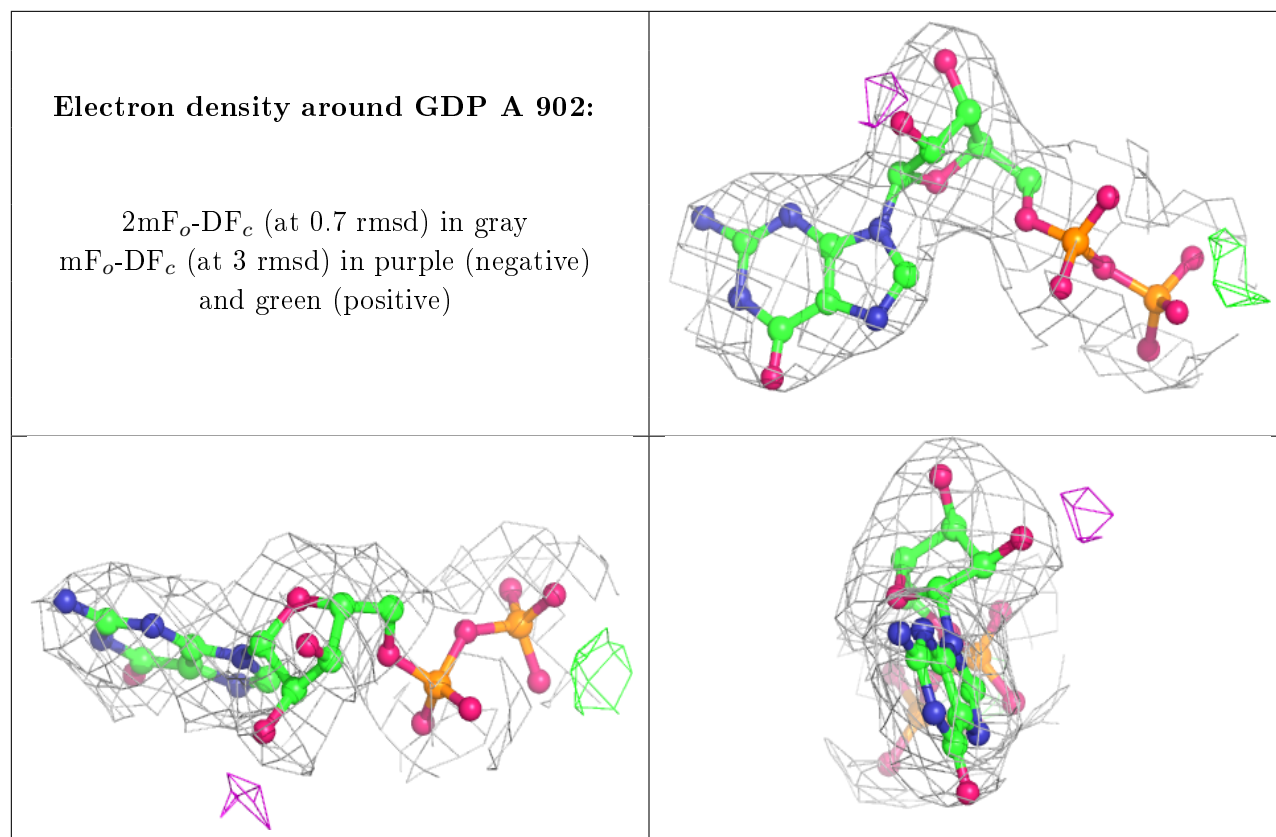
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MOU 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.