Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:07 AM BST

PDB ID	:	1EXV
Title	:	HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH GLCNAC AND CP-403,700
Authors	:	Rath, V.L.; Ammirati, M.; Danley, D.E.; Ekstrom, J.L.; Hynes, T.R.; Olson, T.V.; Hoover, D.J.
Deposited on	:	2000-05-04
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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 ①) were used in the production of this report:

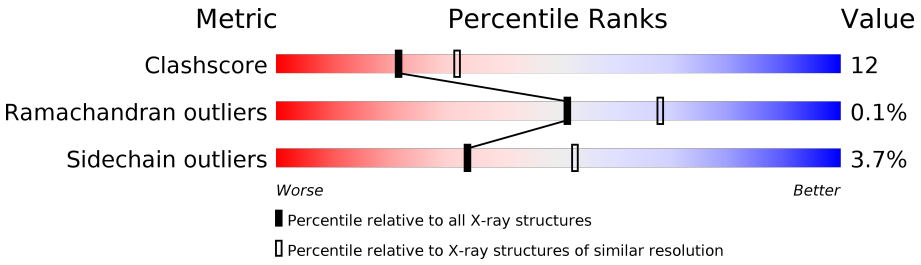
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	67% 24% • 7%
1	B	847	65% 27% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	1901	X	-	-	-
5	MPD	B	1902	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13223 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.

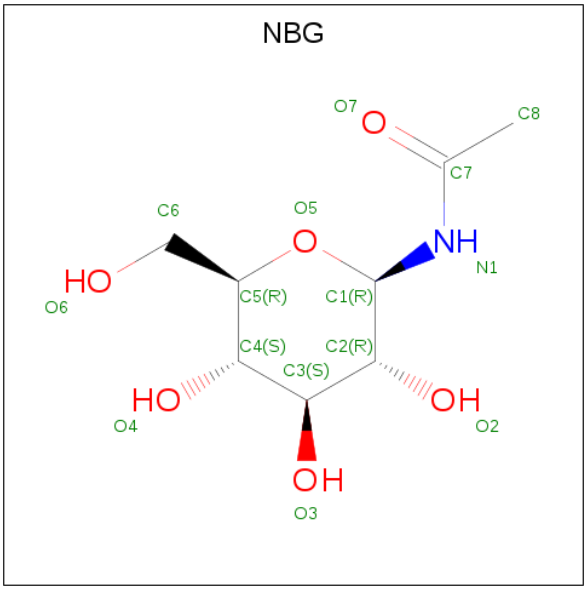
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	786	Total	C	N	O	S	0	0	0
			6377	4098	1083	1167	29			
1	B	786	Total	C	N	O	S	0	0	0
			6377	4098	1083	1167	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	569	ARG	SER	SEE REMARK 999	UNP P06737
B	569	ARG	SER	SEE REMARK 999	UNP P06737

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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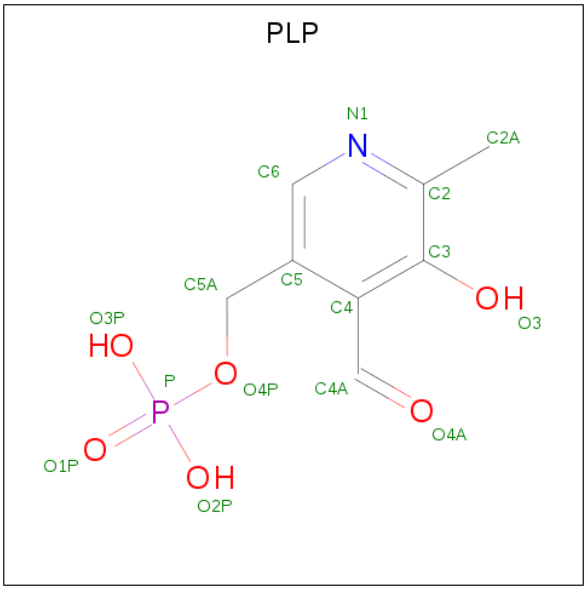
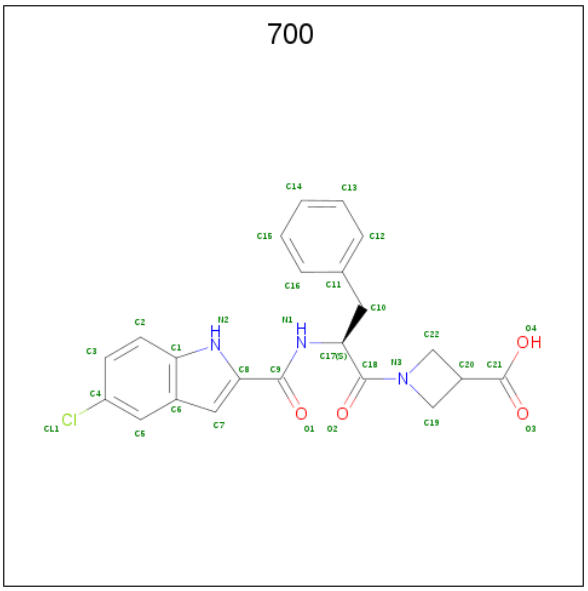
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



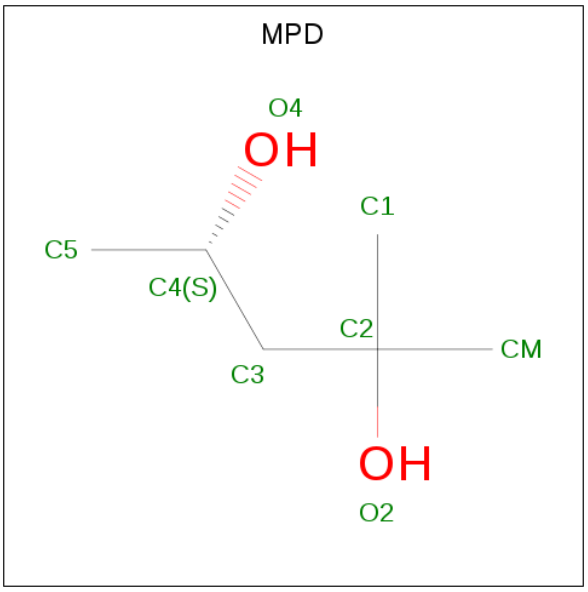
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE -3-CARBOXYLIC ACID (three-letter code: 700) (formula: $C_{22}H_{20}ClN_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	174	Total	O	0	0
			174	174		
6	B	159	Total	O	0	0
			159	159		

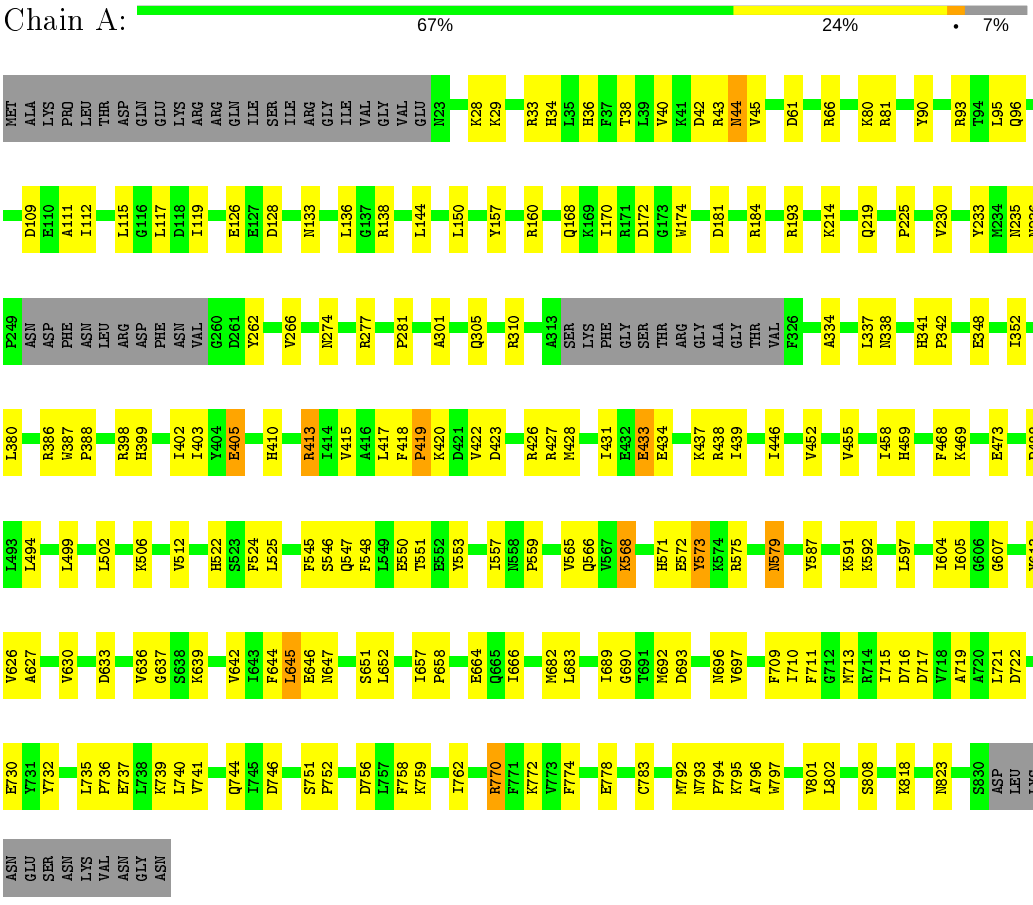
3 Residue-property plots (i)

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

Note EDS was not executed.

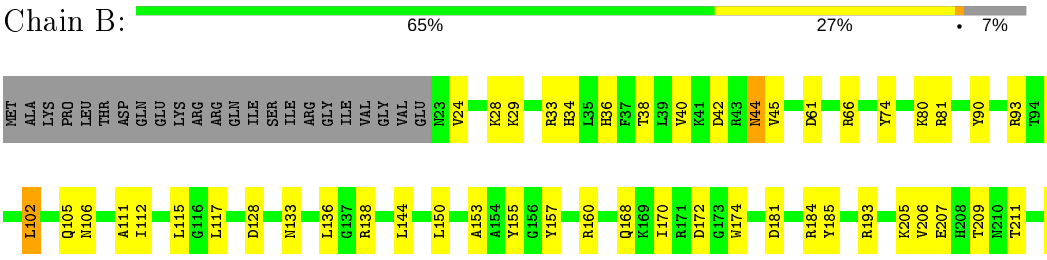
- Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE

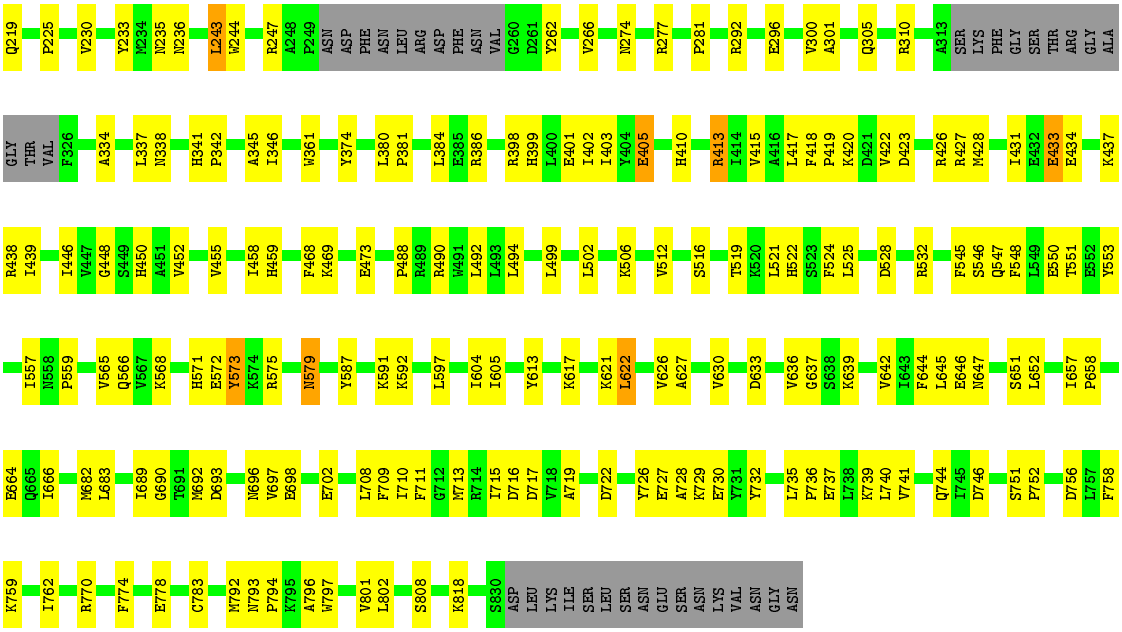
Chain A:



- Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE

Chain B:




Q219 P225 V230 Y233 M234 N235 N236 L243 W244 R247 A248 P249 ASN ASP PHE ASN LEU ARG ASP PHE ASN VAL G260 D261 Y262 V266 N274 R277 P281 R292 E296 V300 A301 Q305 R310 A313 SER LYS PHE GLY SER THR ARG GLY ALA
GLY THR VAL F326 A334 L337 N338 H341 P342 A345 I346 W361 Y374 L380 P381 L384 E385 R386 R398 H399 L400 E401 I402 I403 Y404 E405 H410 R413 I414 V415 A416 L417 F418 P419 K420 D421 V422 D423 R426 R427 M428 I431 E432 E433 E434 K437
R438 I439 I446 V447 G448 S449 H450 A451 V452 V455 I458 H459 F468 K469 E473 P488 R489 R490 W491 L492 L493 L494 L499 L502 K506 V512 S516 T519 K520 L521 H522 S523 F524 L525 D528 R532 F545 S546 Q547 F548 L549 E550 T551 E552 Y553
I557 N558 P559 V565 Q566 V567 K568 H571 E572 Y573 K574 R575 N579 Y587 K591 K592 L597 I604 I605 Y613 K617 K621 L622 V626 A627 V630 D633 V636 G637 S638 K639 V642 I643 F644 L645 E646 N647 S651 L652 I657 P658
E664 Q665 I666 M682 L683 I689 G690 T691 M692 D693 N696 V697 E698 E702 L708 F709 I710 F711 G712 M713 R714 I715 D716 D717 V718 A719 D722 Y726 E727 A728 K729 E730 Y731 Y732 L735 P736 E737 L738 K739 L740 V741 Q744 I745 D746 S751 P752 D756 L757 F758
K759 I762 R770 F774 E778 C783 M792 N793 P794 K795 A796 W797 V801 L802 S808 K818 S830 ASP LEU LYS ILE SER LEU SER ASN GLU SER ASN LYS VAL ASN GLY ASN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.63Å 124.63Å 124.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (99.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.236 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 700, MPD, NBG, PLP

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	0.36	0/6520	0.58	0/8818
1	B	0.35	0/6520	0.58	0/8818
All	All	0.36	0/13040	0.58	0/17636

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6377	0	6372	149	0
1	B	6377	0	6372	159	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	18	0	0
4	B	30	0	18	0	0
5	A	8	0	14	1	0
5	B	8	0	14	0	0
6	A	174	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	159	0	0	12	0
All	All	13223	0	12852	306	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 12.

All (306) 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:96:GLN:HE21	1:A:105:GLN:HE22	1.11	0.98
1:B:96:GLN:HE21	1:B:105:GLN:HE22	1.09	0.98
1:A:168:GLN:HE21	1:A:647:ASN:H	1.21	0.87
1:B:168:GLN:HE21	1:B:647:ASN:H	1.22	0.87
1:B:81:ARG:NH1	1:B:310:ARG:HD3	1.94	0.81
1:A:81:ARG:NH1	1:A:310:ARG:HD3	1.94	0.81
1:B:33:ARG:HD2	6:B:2232:HOH:O	1.80	0.79
1:B:455:VAL:H	1:B:459:HIS:HD2	1.31	0.78
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.67	0.75
1:A:96:GLN:NE2	1:A:105:GLN:HE22	1.84	0.75
1:B:96:GLN:NE2	1:B:105:GLN:HE22	1.82	0.74
1:A:547:GLN:O	1:A:551:THR:HG23	1.89	0.73
1:A:455:VAL:H	1:A:459:HIS:HD2	1.34	0.73
1:B:692:MET:HG3	1:B:697:VAL:HG22	1.69	0.73
1:B:96:GLN:HE21	1:B:105:GLN:NE2	1.86	0.72
1:B:759:LYS:NZ	1:B:759:LYS:HB3	2.05	0.72
1:A:759:LYS:HB3	1:A:759:LYS:NZ	2.06	0.71
1:B:274:ASN:HD22	1:B:277:ARG:HH11	1.40	0.70
1:B:547:GLN:O	1:B:551:THR:HG23	1.91	0.70
1:A:274:ASN:HD22	1:A:277:ARG:HH11	1.39	0.68
1:A:792:MET:O	1:A:794:PRO:HD3	1.94	0.68
1:B:792:MET:O	1:B:794:PRO:HD3	1.93	0.67
1:B:274:ASN:ND2	1:B:277:ARG:HH11	1.93	0.67
1:A:96:GLN:HE21	1:A:105:GLN:NE2	1.91	0.67
1:B:44:ASN:HD22	1:B:45:VAL:N	1.93	0.66
1:A:274:ASN:ND2	1:A:277:ARG:HH11	1.93	0.66
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.31	0.66
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.31	0.65
1:B:66:ARG:HD3	1:B:236:ASN:HA	1.79	0.65
1:A:44:ASN:HD22	1:A:45:VAL:N	1.94	0.64
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.77	0.64
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:HG3	1:A:437:LYS:HE3	1.80	0.63
1:A:66:ARG:HD3	1:A:236:ASN:HA	1.80	0.63
1:B:433:GLU:HG3	1:B:437:LYS:HE3	1.80	0.63
1:A:413:ARG:HE	1:A:413:ARG:HA	1.64	0.62
1:A:571:HIS:HD2	1:A:573:TYR:H	1.49	0.61
1:A:42:ASP:HB2	1:A:44:ASN:HD21	1.66	0.60
1:B:96:GLN:HB2	6:B:2289:HOH:O	2.00	0.60
1:B:727:GLU:HG2	1:B:729:LYS:HG2	1.83	0.60
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.36	0.60
1:B:571:HIS:HD2	1:B:573:TYR:H	1.48	0.60
1:B:630:VAL:O	1:B:636:VAL:HG21	2.02	0.60
1:B:413:ARG:HA	1:B:413:ARG:HE	1.65	0.60
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.84	0.59
1:B:211:THR:OG1	1:B:214:LYS:HE2	2.02	0.59
1:B:546:SER:O	1:B:550:GLU:HG2	2.02	0.59
1:B:732:TYR:CZ	1:B:739:LYS:HG3	2.37	0.59
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.85	0.59
1:B:42:ASP:HB2	1:B:44:ASN:HD21	1.68	0.59
1:A:727:GLU:HG2	1:A:729:LYS:HG2	1.83	0.59
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.85	0.58
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.85	0.58
1:B:28:LYS:HD2	1:B:115:LEU:HG	1.85	0.58
1:A:380:LEU:H	1:A:380:LEU:HD12	1.69	0.58
1:A:732:TYR:CE1	1:A:739:LYS:HA	2.39	0.58
1:A:546:SER:O	1:A:550:GLU:HG2	2.04	0.57
1:B:605:ILE:O	1:B:644:PHE:HA	2.04	0.57
1:A:29:LYS:HE2	1:A:33:ARG:HH21	1.70	0.57
1:A:630:VAL:O	1:A:636:VAL:HG21	2.04	0.57
1:A:28:LYS:HD2	1:A:115:LEU:HG	1.85	0.57
1:B:380:LEU:HD12	1:B:380:LEU:H	1.70	0.57
1:B:45:VAL:HG12	1:B:45:VAL:O	2.05	0.56
1:B:732:TYR:CE1	1:B:739:LYS:HA	2.40	0.56
1:A:386:ARG:HA	1:A:439:ILE:O	2.05	0.56
1:B:386:ARG:HA	1:B:439:ILE:O	2.04	0.56
1:A:93:ARG:O	1:A:490:ARG:NH2	2.38	0.56
1:B:207:GLU:HG2	1:B:209:THR:HG23	1.86	0.56
1:A:770:ARG:HG2	6:A:2155:HOH:O	2.05	0.56
1:B:29:LYS:HE2	1:B:33:ARG:HH21	1.71	0.56
1:A:633:ASP:O	1:A:636:VAL:HG22	2.06	0.56
1:A:525:LEU:HD23	1:A:802:LEU:HD23	1.87	0.55
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:TRP:CH2	1:B:405:GLU:HB3	2.42	0.55
1:B:633:ASP:O	1:B:636:VAL:HG22	2.05	0.55
1:B:93:ARG:O	1:B:490:ARG:NH2	2.39	0.55
1:B:597:LEU:O	1:B:597:LEU:HD12	2.07	0.55
1:A:45:VAL:HG12	1:A:45:VAL:O	2.06	0.55
1:A:597:LEU:HD12	1:A:597:LEU:O	2.07	0.55
1:A:571:HIS:CD2	1:A:573:TYR:H	2.24	0.55
1:A:605:ILE:O	1:A:644:PHE:HA	2.08	0.54
1:A:488:PRO:O	1:A:492:LEU:HB3	2.06	0.54
1:A:689:ILE:O	1:A:689:ILE:HG23	2.08	0.54
1:B:494:LEU:C	1:B:494:LEU:HD23	2.28	0.54
1:A:42:ASP:HB2	1:A:44:ASN:ND2	2.22	0.54
1:B:579:ASN:HD22	1:B:579:ASN:C	2.10	0.54
1:B:301:ALA:O	1:B:305:GLN:HG3	2.08	0.54
1:B:247:ARG:HD2	6:B:2116:HOH:O	2.07	0.53
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.90	0.53
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.90	0.53
1:B:44:ASN:ND2	1:B:45:VAL:HG23	2.23	0.53
1:A:386:ARG:HH21	1:A:438:ARG:HD2	1.73	0.53
1:B:571:HIS:CD2	1:B:573:TYR:H	2.24	0.53
1:A:579:ASN:C	1:A:579:ASN:HD22	2.10	0.53
1:B:488:PRO:O	1:B:492:LEU:HB3	2.08	0.53
1:A:361:TRP:CH2	1:A:405:GLU:HB3	2.44	0.53
1:A:490:ARG:NH1	6:A:2231:HOH:O	2.41	0.53
1:B:235:ASN:O	1:B:236:ASN:HB2	2.08	0.53
1:B:386:ARG:HH21	1:B:438:ARG:HD2	1.73	0.53
1:A:301:ALA:O	1:A:305:GLN:HG3	2.10	0.52
1:A:557:ILE:O	1:A:559:PRO:HD3	2.09	0.52
1:A:565:VAL:HG22	1:A:604:ILE:HB	1.91	0.52
1:B:410:HIS:HE1	1:B:428:MET:O	1.92	0.52
1:B:525:LEU:HD23	1:B:802:LEU:HD23	1.90	0.52
1:A:235:ASN:O	1:A:236:ASN:HB2	2.10	0.52
1:A:455:VAL:H	1:A:459:HIS:CD2	2.23	0.52
1:A:545:PHE:O	1:A:548:PHE:HB3	2.10	0.52
1:A:423:ASP:O	1:A:427:ARG:HB2	2.09	0.52
1:A:494:LEU:HD23	1:A:494:LEU:C	2.30	0.52
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.93	0.52
1:B:575:ARG:HD2	1:B:666:ILE:O	2.09	0.51
1:B:106:ASN:HB3	6:B:2162:HOH:O	2.08	0.51
1:B:708:LEU:HG	6:B:2114:HOH:O	2.09	0.51
1:A:693:ASP:O	1:A:696:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:ILE:HG23	1:B:689:ILE:O	2.11	0.51
1:B:42:ASP:HB2	1:B:44:ASN:ND2	2.25	0.51
1:A:490:ARG:NH1	6:A:2139:HOH:O	2.44	0.51
1:B:181:ASP:OD2	1:B:184:ARG:HB2	2.11	0.51
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.93	0.51
1:B:565:VAL:HG22	1:B:604:ILE:HB	1.93	0.51
1:B:587:TYR:O	1:B:591:LYS:HG2	2.11	0.51
1:B:423:ASP:O	1:B:427:ARG:HB2	2.11	0.50
1:A:410:HIS:HE1	1:A:428:MET:O	1.95	0.50
1:A:737:GLU:O	1:A:741:VAL:HG23	2.11	0.50
1:A:795:LYS:HB2	6:A:2180:HOH:O	2.10	0.50
1:B:262:TYR:O	1:B:266:VAL:HG23	2.11	0.50
1:B:693:ASP:O	1:B:696:ASN:HB2	2.11	0.50
1:B:759:LYS:HZ2	1:B:759:LYS:HB3	1.75	0.50
1:B:341:HIS:HB2	1:B:342:PRO:HD3	1.93	0.50
1:B:557:ILE:O	1:B:559:PRO:HD3	2.11	0.50
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.94	0.50
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.93	0.49
1:A:44:ASN:ND2	1:A:45:VAL:HG23	2.26	0.49
1:B:455:VAL:H	1:B:459:HIS:CD2	2.21	0.49
1:B:545:PHE:O	1:B:548:PHE:HB3	2.12	0.49
1:A:102:LEU:O	1:A:104:LEU:HD13	2.12	0.49
1:A:469:LYS:HG2	1:A:473:GLU:OE2	2.11	0.49
1:A:587:TYR:O	1:A:591:LYS:HG2	2.13	0.49
1:B:174:TRP:CE2	1:B:621:LYS:HG3	2.48	0.49
1:B:24:VAL:HB	6:B:2301:HOH:O	2.13	0.49
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.94	0.49
1:B:732:TYR:CE1	1:B:739:LYS:HG3	2.48	0.49
1:A:422:VAL:HG23	1:A:423:ASP:N	2.27	0.49
1:A:174:TRP:CE2	1:A:621:LYS:HG3	2.48	0.49
1:B:422:VAL:HG23	1:B:423:ASP:N	2.28	0.49
1:A:446:ILE:HD11	1:A:468:PHE:CD2	2.48	0.48
1:A:823:ASN:ND2	6:A:2241:HOH:O	2.46	0.48
1:A:181:ASP:OD2	1:A:184:ARG:HB2	2.13	0.48
1:B:66:ARG:CD	1:B:236:ASN:HA	2.43	0.48
1:A:566:GLN:HB2	1:A:664:GLU:HG3	1.96	0.48
1:B:566:GLN:HB2	1:B:664:GLU:HG3	1.94	0.48
1:B:735:LEU:HD22	1:B:778:GLU:HG3	1.96	0.48
1:A:133:ASN:OD1	1:A:281:PRO:HA	2.14	0.48
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.95	0.48
1:A:715:ILE:HG23	1:A:716:ASP:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:OD1	1:B:281:PRO:HA	2.13	0.48
1:A:399:HIS:O	1:A:403:ILE:HG13	2.14	0.48
1:B:737:GLU:O	1:B:741:VAL:HG23	2.13	0.48
1:B:728:ALA:HB1	1:B:774:PHE:CD1	2.49	0.48
1:A:262:TYR:O	1:A:266:VAL:HG23	2.13	0.48
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.48	0.48
1:B:446:ILE:HD11	1:B:468:PHE:CD2	2.49	0.48
1:B:729:LYS:HG3	1:B:730:GLU:N	2.29	0.48
1:A:735:LEU:HD22	1:A:778:GLU:HG3	1.96	0.48
1:B:185:TYR:HA	6:B:2144:HOH:O	2.14	0.48
1:A:66:ARG:CD	1:A:236:ASN:HA	2.42	0.48
1:A:398:ARG:O	1:A:402:ILE:HG13	2.14	0.47
1:B:170:ILE:CG1	1:B:646:GLU:HG2	2.44	0.47
1:B:740:LEU:O	1:B:744:GLN:HG3	2.14	0.47
1:A:759:LYS:HB3	1:A:759:LYS:HZ3	1.78	0.47
1:B:617:LYS:HD3	6:B:2224:HOH:O	2.14	0.47
1:A:729:LYS:HG3	1:A:730:GLU:N	2.29	0.47
1:A:575:ARG:HD2	1:A:666:ILE:O	2.13	0.47
1:B:206:VAL:HG11	1:B:401:GLU:OE2	2.14	0.47
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.97	0.47
1:B:418:PHE:N	1:B:419:PRO:HD3	2.30	0.47
1:B:469:LYS:HG2	1:B:473:GLU:OE2	2.14	0.47
1:B:636:VAL:O	1:B:639:LYS:HB2	2.15	0.47
1:B:29:LYS:HE2	1:B:33:ARG:NH2	2.29	0.47
1:B:710:ILE:HG22	1:B:711:PHE:N	2.30	0.47
1:A:29:LYS:HE2	1:A:33:ARG:NH2	2.29	0.46
1:B:157:TYR:HD2	1:B:244:TRP:HE1	1.64	0.46
1:B:168:GLN:NE2	1:B:647:ASN:H	2.03	0.46
1:A:28:LYS:HG2	1:A:111:ALA:HB1	1.96	0.46
1:A:636:VAL:O	1:A:639:LYS:HB2	2.15	0.46
1:B:193:ARG:HB2	1:B:225:PRO:HG2	1.97	0.46
1:B:29:LYS:HB3	1:B:29:LYS:HE2	1.70	0.46
1:B:746:ASP:HB2	1:B:762:ILE:HG13	1.96	0.46
1:A:728:ALA:HB1	1:A:774:PHE:CD1	2.51	0.46
1:B:431:ILE:HG22	1:B:433:GLU:OE1	2.14	0.46
1:A:746:ASP:HB2	1:A:762:ILE:HG13	1.97	0.46
1:A:522:HIS:O	1:A:525:LEU:HG	2.16	0.46
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.55	0.46
1:B:715:ILE:HG23	1:B:716:ASP:N	2.31	0.46
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.96	0.46
1:B:28:LYS:HG2	1:B:111:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLU:HB3	6:A:2147:HOH:O	2.16	0.46
1:B:627:ALA:HA	1:B:642:VAL:HB	1.98	0.46
1:A:418:PHE:N	1:A:419:PRO:HD3	2.30	0.45
1:A:29:LYS:HB3	1:A:29:LYS:HE2	1.74	0.45
1:A:690:GLY:O	1:A:710:ILE:HA	2.16	0.45
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.49	0.45
1:B:399:HIS:O	1:B:403:ILE:HG13	2.16	0.45
1:A:168:GLN:NE2	6:A:2007:HOH:O	2.49	0.45
1:A:721:LEU:HD23	1:A:772:LYS:HD3	1.98	0.45
1:B:434:GLU:CD	1:B:434:GLU:H	2.21	0.45
1:B:181:ASP:OD2	1:B:184:ARG:NE	2.49	0.45
1:B:415:VAL:C	1:B:417:LEU:H	2.20	0.45
1:A:431:ILE:HG22	1:A:433:GLU:OE1	2.17	0.44
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.57	0.44
1:A:281:PRO:HG3	1:B:262:TYR:CE2	2.52	0.44
1:B:133:ASN:HB2	6:B:2025:HOH:O	2.16	0.44
1:B:682:MET:HG2	1:B:808:SER:HB3	1.99	0.44
1:B:150:LEU:HD21	1:B:818:LYS:HG3	1.99	0.44
1:A:136:LEU:HD11	1:A:338:ASN:ND2	2.32	0.44
1:A:170:ILE:CG1	1:A:646:GLU:HG2	2.47	0.44
1:A:168:GLN:NE2	1:A:647:ASN:H	2.02	0.44
1:A:740:LEU:O	1:A:744:GLN:HG3	2.17	0.44
1:B:98:THR:O	1:B:102:LEU:HB2	2.18	0.44
1:B:797:TRP:O	1:B:801:VAL:HG23	2.17	0.44
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.64	0.44
1:A:719:ALA:O	1:A:722:ASP:HB2	2.17	0.44
1:B:690:GLY:O	1:B:710:ILE:HA	2.18	0.44
1:A:415:VAL:C	1:A:417:LEU:H	2.21	0.44
1:A:627:ALA:HA	1:A:642:VAL:HB	2.00	0.44
1:A:571:HIS:CD2	1:A:572:GLU:N	2.86	0.44
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.85	0.44
1:A:759:LYS:HB3	1:A:759:LYS:HZ2	1.79	0.44
1:B:233:TYR:CE2	1:B:512:VAL:HG11	2.53	0.44
1:B:398:ARG:O	1:B:402:ILE:HG13	2.18	0.44
1:B:522:HIS:O	1:B:525:LEU:HG	2.17	0.44
1:B:553:TYR:CD1	1:B:553:TYR:N	2.86	0.44
1:B:136:LEU:HD11	1:B:338:ASN:ND2	2.33	0.43
1:A:193:ARG:NH1	5:A:1901:MPD:HM2	2.33	0.43
1:B:528:ASP:O	1:B:532:ARG:HD3	2.19	0.43
1:A:128:ASP:OD2	1:A:651:SER:HB3	2.18	0.43
1:A:710:ILE:HG22	1:A:711:PHE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:LEU:HA	1:B:758:PHE:CZ	2.53	0.43
1:A:387:TRP:HA	1:A:388:PRO:HD3	1.89	0.43
1:A:553:TYR:CD1	1:A:553:TYR:N	2.86	0.43
1:B:44:ASN:HD22	1:B:44:ASN:C	2.19	0.43
1:B:450:HIS:HE1	6:B:2193:HOH:O	2.00	0.43
1:B:719:ALA:O	1:B:722:ASP:HB2	2.18	0.43
1:B:128:ASP:OD2	1:B:651:SER:HB3	2.19	0.43
1:B:36:HIS:O	1:B:40:VAL:HA	2.19	0.43
1:B:571:HIS:CD2	1:B:572:GLU:N	2.86	0.43
1:B:726:TYR:OH	1:B:774:PHE:HB2	2.19	0.43
1:A:622:LEU:HA	1:A:758:PHE:CZ	2.54	0.43
1:B:735:LEU:HA	1:B:736:PRO:HD2	1.86	0.43
1:A:636:VAL:HG23	1:A:637:GLY:N	2.33	0.42
1:A:434:GLU:H	1:A:434:GLU:CD	2.22	0.42
1:B:138:ARG:HD2	1:B:138:ARG:HA	1.90	0.42
1:A:568:LYS:O	1:A:607:GLY:HA3	2.19	0.42
1:A:36:HIS:O	1:A:40:VAL:HA	2.19	0.42
1:B:417:LEU:C	1:B:419:PRO:HD3	2.40	0.42
1:A:138:ARG:HA	1:A:138:ARG:HD2	1.92	0.42
1:A:44:ASN:HD22	1:A:44:ASN:C	2.19	0.42
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.20	0.42
1:A:622:LEU:O	1:A:626:VAL:HG23	2.19	0.42
1:A:682:MET:HG2	1:A:808:SER:HB3	2.01	0.42
1:A:793:ASN:ND2	1:A:796:ALA:HB2	2.35	0.42
1:B:636:VAL:HG23	1:B:637:GLY:N	2.33	0.42
1:B:792:MET:C	1:B:794:PRO:HD3	2.39	0.42
1:A:374:TYR:O	1:A:452:VAL:HA	2.19	0.42
1:B:381:PRO:HA	1:B:384:LEU:HG	2.02	0.42
1:A:797:TRP:O	1:A:801:VAL:HG23	2.20	0.41
1:B:420:LYS:O	1:B:422:VAL:N	2.53	0.41
1:A:417:LEU:C	1:A:419:PRO:HD3	2.41	0.41
1:A:645:LEU:HA	1:A:645:LEU:HD23	1.87	0.41
1:B:205:LYS:HE3	1:B:217:ASP:HB2	2.02	0.41
1:B:374:TYR:O	1:B:452:VAL:HA	2.20	0.41
1:B:711:PHE:HA	6:B:2251:HOH:O	2.19	0.41
1:A:112:ILE:HG23	1:A:117:LEU:HB2	2.02	0.41
1:A:150:LEU:HD21	1:A:818:LYS:HG3	2.02	0.41
1:A:144:LEU:HB3	1:A:230:VAL:HG11	2.02	0.41
1:A:348:GLU:O	1:A:352:ILE:HG13	2.20	0.41
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.55	0.41
1:B:144:LEU:HB3	1:B:230:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:SER:N	1:A:752:PRO:HD3	2.36	0.41
1:A:42:ASP:CB	1:A:44:ASN:ND2	2.84	0.41
1:B:112:ILE:HG23	1:B:117:LEU:HB2	2.02	0.41
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.56	0.41
1:A:420:LYS:O	1:A:422:VAL:N	2.54	0.41
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.21	0.41
1:B:292:ARG:O	1:B:296:GLU:HG3	2.21	0.41
1:B:458:ILE:HG23	1:B:459:HIS:N	2.36	0.41
1:B:793:ASN:ND2	1:B:796:ALA:HB2	2.35	0.41
1:A:43:ARG:HA	1:A:43:ARG:HD2	1.92	0.41
1:A:458:ILE:HG23	1:A:459:HIS:N	2.35	0.41
1:B:168:GLN:NE2	6:B:2237:HOH:O	2.46	0.41
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.54	0.41
1:B:566:GLN:HG3	1:B:664:GLU:HB2	2.04	0.40
1:B:571:HIS:HD2	1:B:572:GLU:N	2.19	0.40
1:B:622:LEU:O	1:B:626:VAL:HG23	2.21	0.40
1:A:792:MET:C	1:A:794:PRO:HD3	2.41	0.40
1:B:698:GLU:O	1:B:702:GLU:HG2	2.21	0.40
1:B:751:SER:N	1:B:752:PRO:HD3	2.36	0.40
1:B:300:VAL:HG13	1:B:345:ALA:HA	2.03	0.40
1:B:521:LEU:HB3	1:B:802:LEU:HD11	2.03	0.40
1:A:433:GLU:HA	1:A:437:LYS:HG2	2.04	0.40
1:A:262:TYR:CE2	1:B:281:PRO:HG3	2.56	0.40
1:B:433:GLU:HA	1:B:437:LYS:HG2	2.04	0.40
1:A:571:HIS:HD2	1:A:572:GLU:N	2.18	0.40
1:A:579:ASN:ND2	1:A:579:ASN:C	2.75	0.40
1:B:45:VAL:O	1:B:45:VAL:CG1	2.69	0.40
1:B:516:SER:O	1:B:519:THR:HG23	2.22	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	780/847 (92%)	731 (94%)	48 (6%)	1 (0%)	51 68
1	B	780/847 (92%)	730 (94%)	50 (6%)	0	100 100
All	All	1560/1694 (92%)	1461 (94%)	98 (6%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	PRO

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	687/740 (93%)	661 (96%)	26 (4%)	33 51
1	B	687/740 (93%)	662 (96%)	25 (4%)	35 54
All	All	1374/1480 (93%)	1323 (96%)	51 (4%)	34 53

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	172	ASP
1	A	214	LYS
1	A	219	GLN
1	A	243	LEU
1	A	337	LEU
1	A	405	GLU
1	A	413	ARG
1	A	426	ARG
1	A	433	GLU
1	A	499	LEU
1	A	502	LEU

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Mol	Chain	Res	Type
1	A	568	LYS
1	A	573	TYR
1	A	579	ASN
1	A	592	LYS
1	A	613	TYR
1	A	622	LEU
1	A	645	LEU
1	A	652	LEU
1	A	683	LEU
1	A	756	ASP
1	A	770	ARG
1	B	44	ASN
1	B	90	TYR
1	B	95	LEU
1	B	102	LEU
1	B	172	ASP
1	B	219	GLN
1	B	243	LEU
1	B	337	LEU
1	B	405	GLU
1	B	413	ARG
1	B	426	ARG
1	B	433	GLU
1	B	499	LEU
1	B	502	LEU
1	B	568	LYS
1	B	573	TYR
1	B	579	ASN
1	B	592	LYS
1	B	613	TYR
1	B	622	LEU
1	B	645	LEU
1	B	652	LEU
1	B	683	LEU
1	B	756	ASP
1	B	770	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	34	HIS

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Mol	Chain	Res	Type
1	A	44	ASN
1	A	96	GLN
1	A	97	ASN
1	A	114	GLN
1	A	167	ASN
1	A	168	GLN
1	A	236	ASN
1	A	239	ASN
1	A	270	ASN
1	A	274	ASN
1	A	284	ASN
1	A	305	GLN
1	A	369	GLN
1	A	410	HIS
1	A	459	HIS
1	A	481	ASN
1	A	541	ASN
1	A	566	GLN
1	A	571	HIS
1	A	579	ASN
1	A	823	ASN
1	B	23	ASN
1	B	32	ASN
1	B	34	HIS
1	B	44	ASN
1	B	62	HIS
1	B	96	GLN
1	B	114	GLN
1	B	167	ASN
1	B	168	GLN
1	B	236	ASN
1	B	239	ASN
1	B	270	ASN
1	B	274	ASN
1	B	284	ASN
1	B	305	GLN
1	B	369	GLN
1	B	410	HIS
1	B	450	HIS
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN

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Mol	Chain	Res	Type
1	B	566	GLN
1	B	571	HIS
1	B	579	ASN
1	B	747	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NBG	A	861	-	15,15,15	1.44	3 (20%)	21,21,21	1.20	1 (4%)
3	PLP	A	860	1	15,15,16	1.49	1 (6%)	20,22,23	1.47	5 (25%)
4	700	A	862	-	28,33,33	2.60	8 (28%)	32,47,47	1.60	5 (15%)
3	PLP	B	1860	1	15,15,16	1.81	2 (13%)	20,22,23	1.40	4 (20%)
5	MPD	A	1901	-	7,7,7	0.50	0	9,10,10	0.75	0
4	700	B	1862	-	28,33,33	2.61	13 (46%)	32,47,47	1.53	5 (15%)
5	MPD	B	1902	-	7,7,7	0.74	0	9,10,10	0.72	0
2	NBG	B	1861	-	15,15,15	1.68	3 (20%)	21,21,21	1.36	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
3	PLP	A	860	1	-	1/6/6/8	0/1/1/1
4	700	A	862	-	-	0/15/32/32	0/4/4/4
3	PLP	B	1860	1	-	2/6/6/8	0/1/1/1
5	MPD	A	1901	-	1/1/2/2	1/5/5/5	-
4	700	B	1862	-	-	0/15/32/32	0/4/4/4
5	MPD	B	1902	-	1/1/2/2	1/5/5/5	-
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	862	700	C7-C8	7.15	1.52	1.39
4	B	1862	700	C7-C8	6.96	1.52	1.39
4	A	862	700	C22-C20	6.03	1.60	1.55
3	B	1860	PLP	C4A-C4	-5.55	1.40	1.51
4	B	1862	700	C22-C20	5.37	1.60	1.55
4	B	1862	700	C17-C18	-5.05	1.43	1.53
4	A	862	700	C17-C18	-4.55	1.44	1.53
3	A	860	PLP	C4A-C4	-4.52	1.42	1.51
2	B	1861	NBG	C2-C1	4.21	1.57	1.52
4	A	862	700	C5-C4	3.68	1.43	1.36
2	A	861	NBG	C2-C1	3.47	1.56	1.52
4	B	1862	700	C3-C4	3.30	1.44	1.38
4	B	1862	700	C5-C4	3.19	1.42	1.36
4	B	1862	700	C2-C3	3.16	1.43	1.36
4	A	862	700	C2-C3	2.91	1.42	1.36
2	B	1861	NBG	C1-N1	2.89	1.46	1.43
4	A	862	700	C7-C6	2.74	1.51	1.41
4	A	862	700	C3-C4	2.49	1.42	1.38
4	B	1862	700	C12-C11	2.45	1.44	1.38
4	A	862	700	C12-C11	2.42	1.44	1.38
4	B	1862	700	C7-C6	2.41	1.50	1.41
2	B	1861	NBG	C4-C5	2.33	1.57	1.53
2	A	861	NBG	C1-N1	2.32	1.46	1.43
2	A	861	NBG	C3-C2	2.31	1.58	1.52
4	B	1862	700	C16-C11	2.22	1.43	1.38
4	B	1862	700	C9-N1	2.20	1.39	1.34
3	B	1860	PLP	C3-C2	-2.20	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	700	C13-C12	2.13	1.43	1.38
4	B	1862	700	C10-C17	2.12	1.59	1.54
4	B	1862	700	C10-C11	2.08	1.56	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1861	NBG	C5-O5-C1	4.37	118.44	112.52
4	A	862	700	C8-N2-C1	4.33	113.47	104.45
4	A	862	700	C8-C9-N1	4.31	123.20	115.20
4	B	1862	700	C8-N2-C1	4.11	113.02	104.45
4	B	1862	700	C8-C9-N1	3.96	122.56	115.20
2	A	861	NBG	C5-O5-C1	3.92	117.83	112.52
4	A	862	700	C7-C6-C1	-3.37	103.33	106.27
3	A	860	PLP	O3P-P-O4P	-3.09	98.51	106.73
4	B	1862	700	C7-C6-C1	-3.01	103.65	106.27
4	A	862	700	O1-C9-C8	-2.61	115.39	121.08
3	A	860	PLP	O3P-P-O2P	2.58	117.49	107.64
4	B	1862	700	C3-C2-C1	-2.50	117.69	120.84
4	B	1862	700	O1-C9-C8	-2.40	115.86	121.08
3	A	860	PLP	C6-C5-C4	2.40	120.05	118.16
2	B	1861	NBG	C2-C1-N1	-2.34	108.55	111.30
3	B	1860	PLP	O4P-P-O1P	-2.33	99.92	106.47
3	B	1860	PLP	C6-C5-C4	2.23	119.92	118.16
3	B	1860	PLP	O2P-P-O4P	-2.19	100.91	106.73
4	A	862	700	C3-C2-C1	-2.15	118.13	120.84
3	B	1860	PLP	C2A-C2-C3	2.06	123.44	120.89
3	A	860	PLP	C2A-C2-C3	2.05	123.42	120.89
3	A	860	PLP	O4P-C5A-C5	-2.03	105.48	109.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1901	MPD	C4
5	B	1902	MPD	C4

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	860	PLP	C4-C5-C5A-O4P
3	B	1860	PLP	C5A-O4P-P-O1P
5	A	1901	MPD	C2-C3-C4-O4

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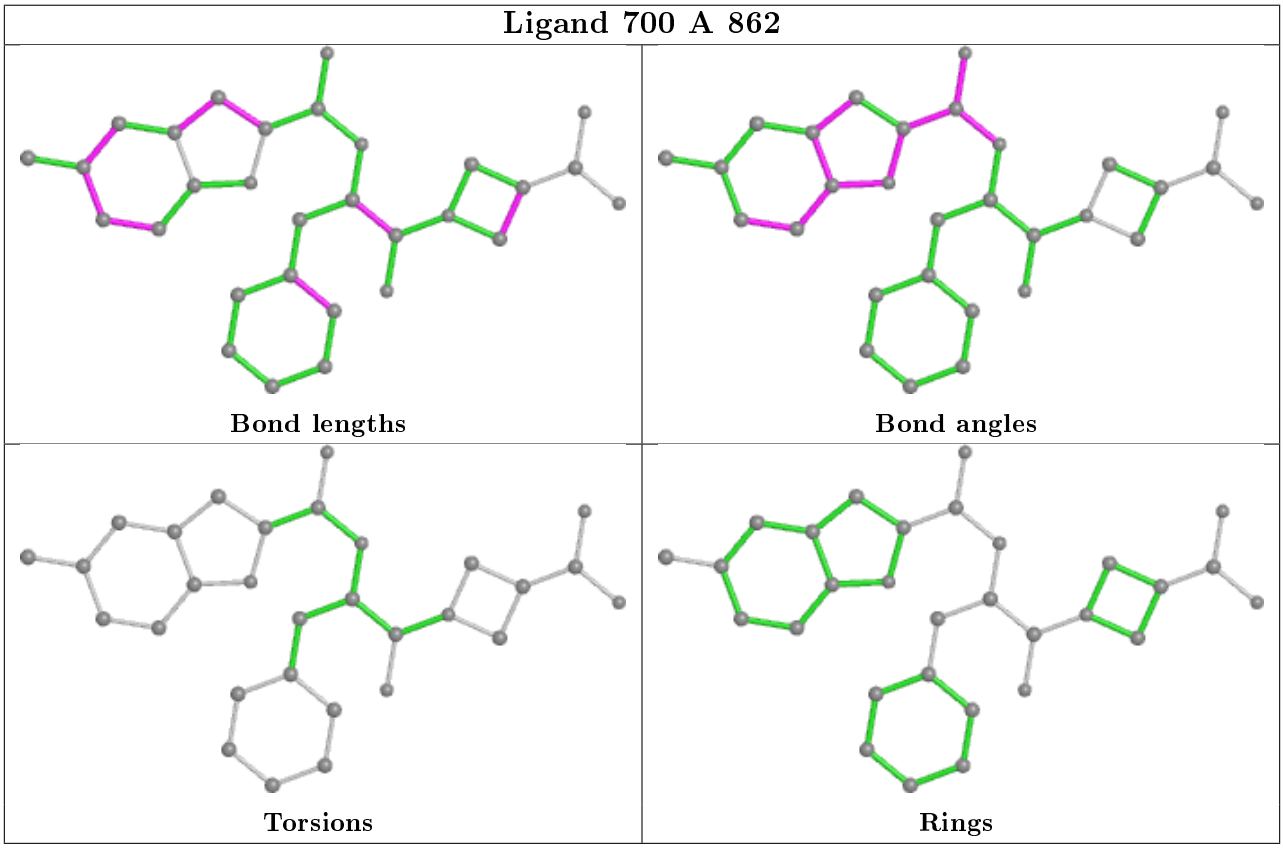
Mol	Chain	Res	Type	Atoms
5	B	1902	MPD	C2-C3-C4-C5
3	B	1860	PLP	C5A-O4P-P-O2P

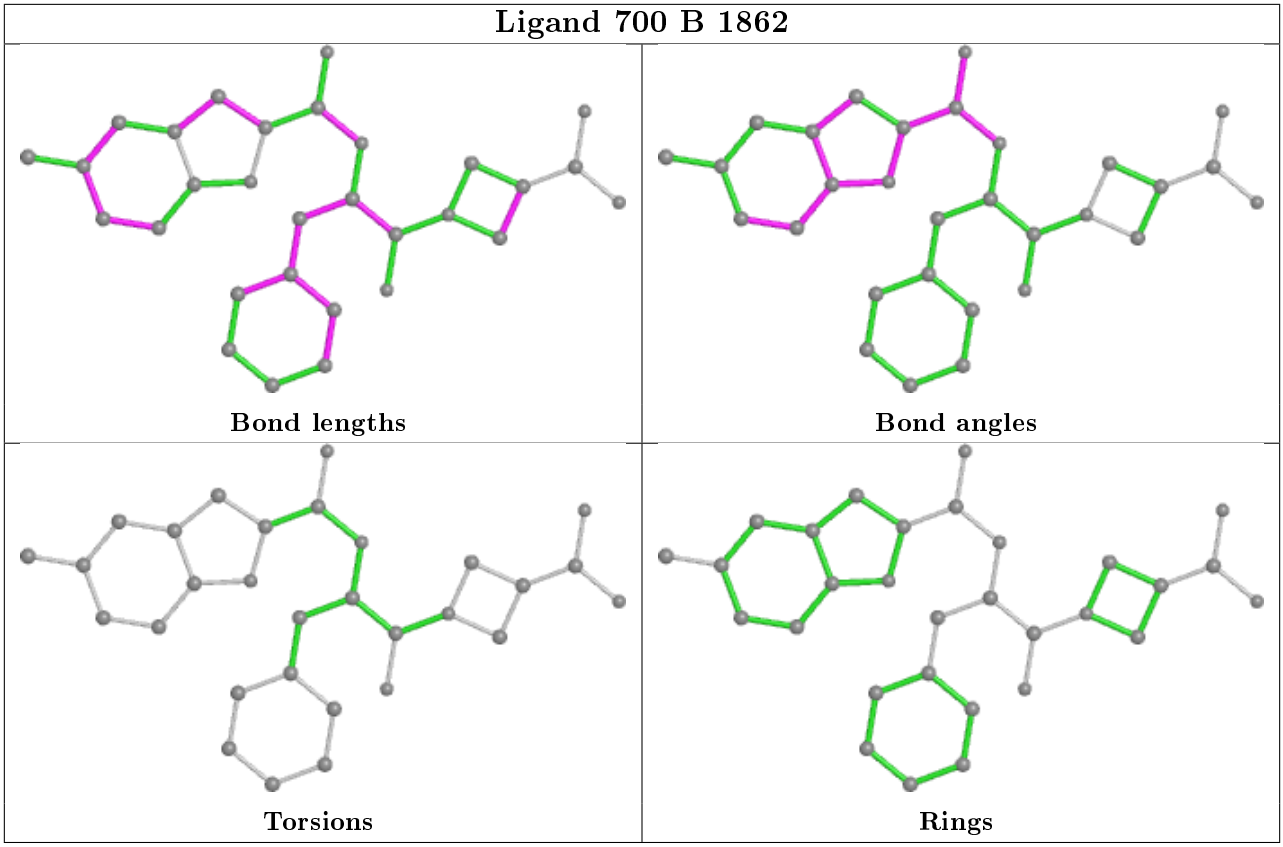
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1901	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.