



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:30 AM UTC

PDB ID : 2JID / pdb_00002jid
Title : Human Dipeptidyl peptidase IV in complex with 1-(3,4-Dimethoxy-phenyl) -
3-m-tolyl-piperidine-4-ylamine
Authors : Hennig, M.; Stihle, M.; Luebbbers, T.; Thoma, R.
Deposited on : 2007-02-28
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

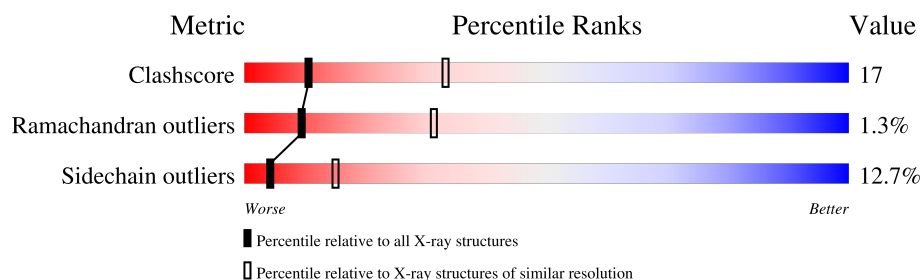
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	736	
1	B	736	

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
2	NAG	B	1770	X	-	-	-

2 Entry composition [i](#)

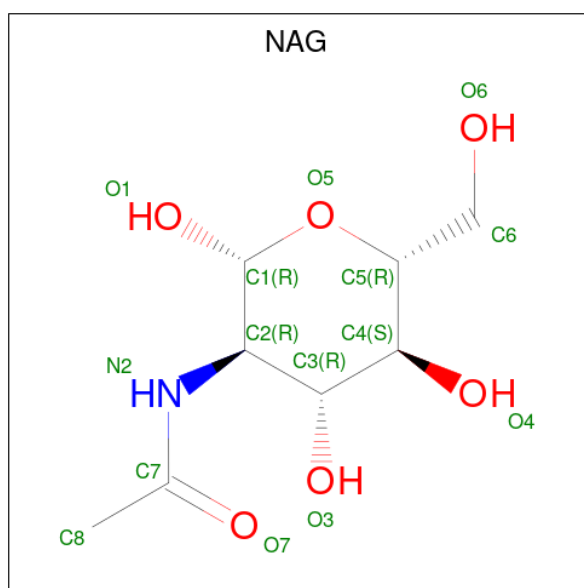
There are 4 unique types of molecules in this entry. The entry contains 12214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIPEPTIDYL PEPTIDASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



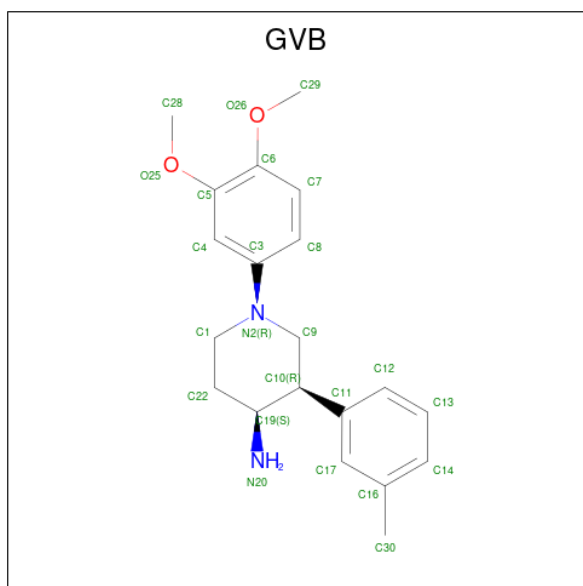
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (3R,4S)-1-(3,4-DIMETHOXYPHENYL)-3-(3-METHYLPHENYL)PIPERIDI
N-4-AMINE (CCD ID: GVB) (formula: C₂₀H₂₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	20	2	2		
3	B	1	Total	C	N	O	0	0
			24	20	2	2		

- Molecule 4 is water.

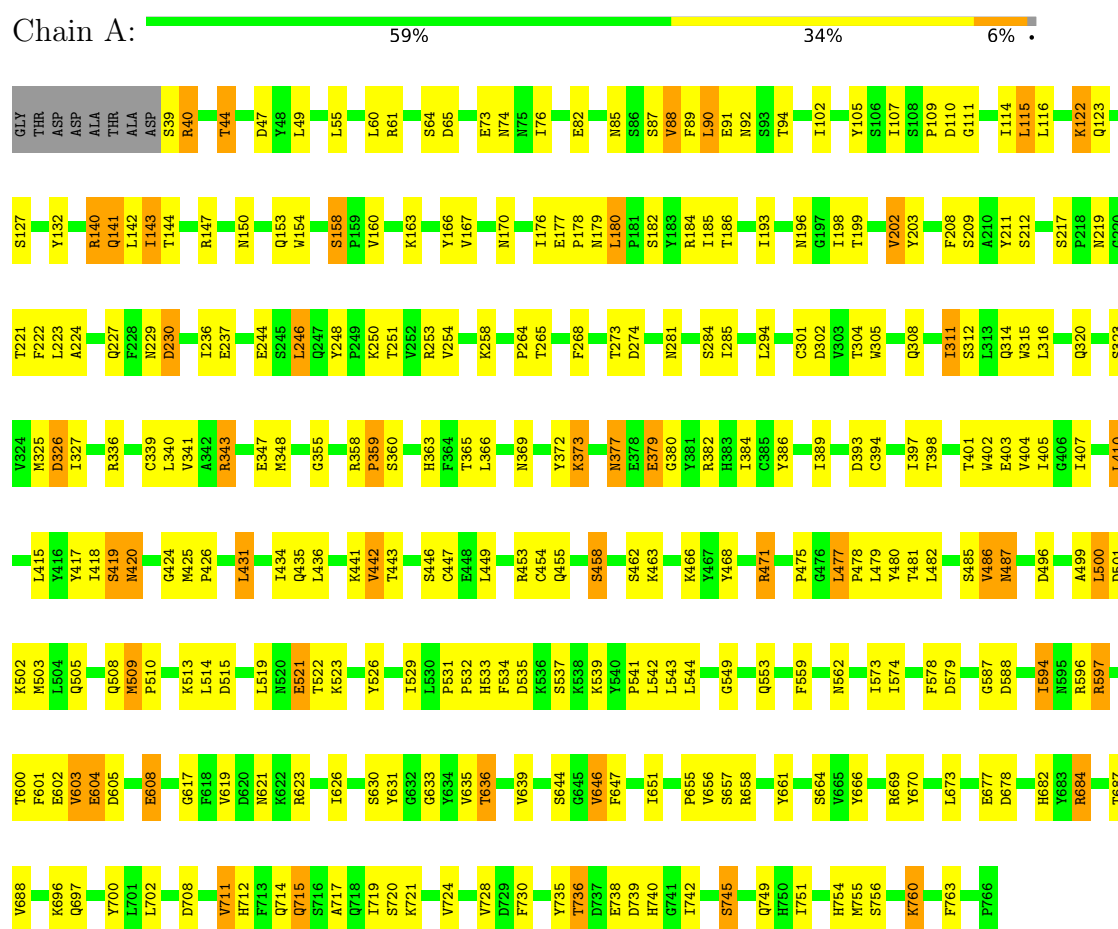
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	73	Total	O	0	0
			73	73		

3 Residue-property plots

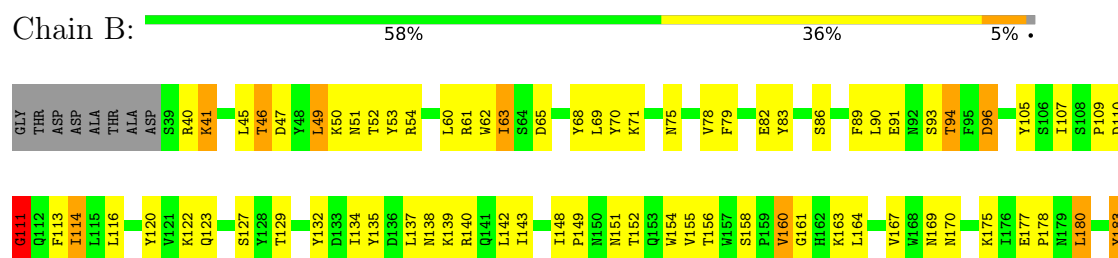
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: DIPEPTIDYL PEPTIDASE 4



• Molecule 1: DIPEPTIDYL PEPTIDASE 4





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.25Å 66.82Å 423.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.4 (20.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12214	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: GVB, NAG

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	0.78	0/6135	1.04	19/8344 (0.2%)
1	B	0.82	2/6135 (0.0%)	1.03	10/8344 (0.1%)
All	All	0.80	2/12270 (0.0%)	1.04	29/16688 (0.2%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	558	VAL	CA-CB	6.13	1.62	1.54
1	B	319	ILE	CA-CB	5.08	1.58	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	597	ARG	N-CA-C	7.35	119.08	110.41
1	A	454	CYS	N-CA-C	6.84	119.56	108.34
1	B	540	TYR	N-CA-C	6.69	119.14	109.84
1	A	562	ASN	N-CA-C	6.45	116.57	108.45
1	B	96	ASP	N-CA-C	-6.44	105.39	113.18
1	A	442	VAL	CB-CA-C	-6.32	101.42	110.83
1	A	458	SER	N-CA-C	-6.31	99.48	109.07
1	A	509	MET	CA-C-N	-6.29	114.15	120.31
1	A	509	MET	C-N-CA	-6.29	114.15	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ILE	N-CA-C	-6.29	107.74	113.71
1	A	202	VAL	CB-CA-C	-6.23	103.73	112.14
1	A	141	GLN	N-CA-C	6.13	118.68	108.13
1	B	350	THR	N-CA-C	-5.98	106.14	113.50
1	B	594	ILE	N-CA-C	-5.83	107.06	112.83
1	A	521	GLU	N-CA-C	-5.78	104.94	113.61
1	B	111	GLY	N-CA-C	5.70	126.68	113.18
1	B	562	ASN	N-CA-C	5.56	118.93	108.65
1	B	616	MET	N-CA-C	-5.46	99.78	109.06
1	A	487	ASN	N-CA-C	-5.39	98.85	108.13
1	A	711	VAL	CB-CA-C	-5.29	106.19	111.80
1	B	327	ILE	N-CA-C	5.20	115.56	107.28
1	A	477	LEU	CA-C-N	5.20	126.33	119.84
1	A	477	LEU	C-N-CA	5.20	126.33	119.84
1	B	558	VAL	N-CA-C	5.16	116.66	109.55
1	A	193	ILE	N-CA-C	5.13	115.67	111.62
1	B	360	SER	N-CA-C	5.09	117.10	110.53
1	A	87	SER	N-CA-C	5.06	116.21	108.42
1	A	468	TYR	N-CA-C	5.03	117.36	108.75
1	A	664	SER	N-CA-C	5.02	116.44	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5684	207	0
1	B	5963	0	5681	199	0
2	A	56	0	52	10	0
2	B	56	0	52	3	0
3	A	24	0	26	3	0
3	B	24	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	55	0	0	5	0
4	B	73	0	0	4	0
All	All	12214	0	11521	396	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 17.

All (396) 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:B:229:ASN:HD21	2:B:1769:NAG:C1	1.47	1.26
1:A:281:ASN:HD21	2:A:1769:NAG:C1	1.51	1.23
1:B:351:THR:HG22	1:B:592:HIS:ND1	1.67	1.09
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.30	1.07
1:A:608:GLU:HA	1:A:608:GLU:OE1	1.51	1.02
1:B:600:THR:HG23	1:B:601:PHE:H	1.26	1.01
1:A:696:LYS:HE2	1:A:697:GLN:HE21	1.26	1.00
1:A:196:ASN:OD1	1:A:227:GLN:HG3	1.65	0.97
1:A:756:SER:O	1:A:760:LYS:HG3	1.65	0.97
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.47	0.94
1:B:229:ASN:ND2	2:B:1769:NAG:C1	2.31	0.93
1:A:40:ARG:H	1:A:40:ARG:HH11	1.10	0.92
1:A:281:ASN:ND2	2:A:1769:NAG:C1	2.35	0.89
1:B:403:GLU:H	1:B:420:ASN:HD21	1.20	0.89
1:A:751:ILE:HG12	1:A:755:MET:HE2	1.53	0.89
1:B:597:ARG:O	1:B:600:THR:HG22	1.71	0.89
1:A:140:ARG:HG3	1:A:140:ARG:HH11	1.38	0.88
1:A:720:SER:O	1:A:724:VAL:HG23	1.77	0.85
1:A:85:ASN:HD21	2:A:1768:NAG:C1	1.89	0.84
1:B:41:LYS:HE2	1:B:53:TYR:OH	1.78	0.83
1:B:82:GLU:HG3	1:B:83:TYR:CE2	2.14	0.82
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.62	0.81
1:A:82:GLU:HG2	4:A:2008:HOH:O	1.80	0.81
1:A:312:SER:OG	1:A:325:MET:HE3	1.81	0.80
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.63	0.80
1:A:40:ARG:HH11	1:A:40:ARG:N	1.81	0.79
1:A:745:SER:O	1:A:749:GLN:HG3	1.82	0.78
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.84	0.78
1:A:85:ASN:HD21	2:A:1768:NAG:C2	1.97	0.78
1:B:312:SER:OG	1:B:325:MET:HE3	1.84	0.77
1:A:377:ASN:C	1:A:377:ASN:HD22	1.93	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:THR:HG23	1:B:601:PHE:N	1.99	0.75
1:A:40:ARG:H	1:A:40:ARG:NH1	1.83	0.75
1:B:648:LYS:HE3	1:B:762:CYS:O	1.86	0.75
1:B:611:ARG:O	1:B:614:SER:HB2	1.87	0.74
1:A:44:THR:HG22	1:A:47:ASP:H	1.52	0.74
1:A:477:LEU:CD1	1:A:501:ASP:HB2	2.17	0.74
1:A:714:GLN:NE2	1:B:249:PRO:HD3	2.03	0.74
1:A:85:ASN:HD21	2:A:1768:NAG:H2	1.54	0.73
1:B:122:LYS:HE3	4:B:2012:HOH:O	1.88	0.71
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.72	0.71
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.74	0.70
1:B:175:LYS:NZ	1:B:180:LEU:O	2.25	0.70
1:A:150:ASN:HD21	2:A:1767:NAG:C1	2.05	0.70
1:A:140:ARG:HG3	1:A:140:ARG:NH1	2.01	0.69
1:B:45:LEU:HG	1:B:49:LEU:CD2	2.19	0.69
1:A:74:ASN:C	1:A:92:ASN:HB3	2.18	0.68
1:A:326:ASP:OD2	1:A:339:CYS:HB3	1.92	0.68
1:B:194:ILE:HD12	2:B:1769:NAG:H82	1.76	0.68
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.75	0.68
1:A:696:LYS:HG3	1:A:697:GLN:HG3	1.74	0.68
1:A:229:ASN:HB3	1:A:265:THR:OG1	1.94	0.68
1:A:39:SER:N	1:A:508:GLN:HG2	2.09	0.68
1:A:147:ARG:HD2	2:A:1767:NAG:H81	1.74	0.68
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.29	0.68
1:B:293:MET:HE2	1:B:324:VAL:HG23	1.77	0.67
1:A:327:ILE:HD12	1:A:343:ARG:HB2	1.77	0.66
1:B:464:GLU:HA	4:B:2042:HOH:O	1.94	0.66
1:A:44:THR:HB	1:A:47:ASP:OD2	1.95	0.66
1:A:688:VAL:HG11	1:A:719:ILE:HD13	1.78	0.66
1:A:386:TYR:O	1:A:394:CYS:HB2	1.97	0.65
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.78	0.65
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.77	0.65
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.27	0.65
1:B:351:THR:CG2	1:B:592:HIS:ND1	2.53	0.65
1:A:403:GLU:H	1:A:420:ASN:HD21	1.45	0.64
1:A:150:ASN:HD21	2:A:1767:NAG:C2	2.10	0.64
1:A:85:ASN:ND2	2:A:1768:NAG:C1	2.61	0.64
1:B:143:ILE:HG13	1:B:143:ILE:O	1.97	0.64
1:A:531:PRO:HD2	1:A:534:PHE:HD1	1.63	0.63
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.14	0.63
1:A:509:MET:HE3	1:A:510:PRO:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:C	1:B:377:ASN:HD22	2.07	0.63
1:B:403:GLU:H	1:B:420:ASN:ND2	1.94	0.62
1:B:657:SER:H	1:B:715:GLN:NE2	1.97	0.62
1:B:221:THR:O	1:B:273:THR:HG22	2.00	0.62
1:B:597:ARG:O	1:B:600:THR:CG2	2.46	0.62
1:A:153:GLN:HB3	1:A:211:TYR:CE2	2.35	0.61
1:B:377:ASN:ND2	1:B:381:TYR:H	1.98	0.61
1:B:414:TYR:CD1	1:B:433:LYS:HE2	2.35	0.61
1:A:446:SER:HA	1:A:449:LEU:HD12	1.82	0.61
1:B:247:GLN:HG2	1:B:248:TYR:CD1	2.36	0.61
1:A:658:ARG:HG3	1:A:687:THR:HG22	1.83	0.61
1:A:237:GLU:OE2	1:A:253:ARG:CD	2.49	0.60
1:A:237:GLU:OE2	1:A:253:ARG:HD3	2.01	0.60
1:B:415:LEU:HD23	1:B:416:TYR:N	2.17	0.60
1:A:320:GLN:OE1	1:A:669:ARG:HG3	2.02	0.59
1:A:340:LEU:HD22	1:A:343:ARG:HH11	1.68	0.59
1:B:482:LEU:HD23	1:B:492:ARG:HH12	1.66	0.59
1:B:377:ASN:HD21	1:B:381:TYR:H	1.50	0.59
1:B:40:ARG:HB3	1:B:506:ASN:O	2.02	0.59
1:B:193:ILE:HG22	1:B:194:ILE:CG1	2.20	0.59
1:A:61:ARG:HB3	4:A:2005:HOH:O	2.01	0.59
1:B:138:ASN:C	1:B:139:LYS:HG3	2.28	0.59
1:A:657:SER:OG	1:A:715:GLN:HB3	2.03	0.58
1:A:55:LEU:HD21	1:A:559:PHE:HE2	1.67	0.58
1:A:535:ASP:OD1	1:A:537:SER:HB3	2.04	0.58
1:A:542:LEU:HD12	1:A:619:VAL:HG21	1.86	0.58
1:A:721:LYS:NZ	1:B:242:SER:O	2.33	0.58
1:B:351:THR:HG22	1:B:592:HIS:CG	2.38	0.58
1:A:715:GLN:O	1:A:719:ILE:HG13	2.03	0.58
1:A:728:VAL:O	1:B:750:HIS:HE1	1.86	0.58
1:A:340:LEU:HB2	1:A:343:ARG:HD3	1.86	0.58
1:A:340:LEU:HD22	1:A:343:ARG:NH1	2.19	0.57
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.34	0.57
1:B:600:THR:CG2	1:B:601:PHE:H	2.07	0.57
1:A:603:VAL:HG22	1:A:635:VAL:HG13	1.87	0.56
1:A:384:ILE:HG21	1:A:397:ILE:HD11	1.87	0.56
1:A:717:ALA:HB1	1:B:736:THR:HG23	1.86	0.56
1:A:323:SER:OG	1:A:347:GLU:HB2	2.06	0.56
1:A:74:ASN:HB2	1:A:92:ASN:HB2	1.87	0.56
1:A:594:ILE:HD11	1:A:602:GLU:H	1.71	0.55
1:A:751:ILE:HG12	1:A:755:MET:CE	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:ASN:C	1:B:562:ASN:HD22	2.14	0.55
1:B:598:LEU:O	1:B:682:HIS:HE1	1.89	0.55
1:B:227:GLN:O	1:B:266:VAL:HA	2.07	0.55
1:B:666:TYR:CZ	3:B:1771:GVB:H12	2.41	0.55
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.42	0.55
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.07	0.55
1:A:657:SER:H	1:A:715:GLN:HE21	1.55	0.55
1:A:377:ASN:C	1:A:377:ASN:ND2	2.59	0.55
1:A:735:TYR:O	1:A:736:THR:C	2.49	0.55
1:A:684:ARG:HD3	4:A:2049:HOH:O	2.07	0.54
1:A:115:LEU:CD2	1:A:132:TYR:HD1	2.19	0.54
1:A:714:GLN:HE22	1:B:249:PRO:HD3	1.72	0.54
1:A:199:THR:HG22	1:A:203:TYR:HB3	1.90	0.54
1:B:401:THR:CG2	1:B:401:THR:O	2.55	0.54
1:A:401:THR:O	1:A:401:THR:HG22	2.07	0.54
1:B:517:ILE:HD11	1:B:578:PHE:CE1	2.42	0.54
1:A:597:ARG:O	1:A:600:THR:OG1	2.25	0.54
1:B:177:GLU:HB2	1:B:180:LEU:CD2	2.38	0.54
1:B:621:ASN:HA	1:B:624:ILE:HD11	1.91	0.53
1:B:195:TYR:HB2	1:B:228:PHE:HB2	1.89	0.53
1:B:675:THR:O	1:B:680:LEU:HB2	2.09	0.53
1:A:153:GLN:HB3	1:A:211:TYR:HE2	1.71	0.53
1:A:738:GLU:OE1	1:A:742:ILE:HA	2.09	0.53
1:A:219:ASN:HB2	1:A:308:GLN:OE1	2.08	0.53
1:A:700:TYR:OH	1:A:702:LEU:HD13	2.09	0.53
1:B:341:VAL:O	1:B:343:ARG:N	2.41	0.53
1:A:122:LYS:HG3	1:A:123:GLN:N	2.24	0.53
1:B:372:TYR:CE2	1:B:386:TYR:CD1	2.97	0.53
1:A:531:PRO:HD2	1:A:534:PHE:CD1	2.43	0.52
1:B:658:ARG:HH22	1:B:684:ARG:HH21	1.56	0.52
1:A:658:ARG:HG3	1:A:687:THR:CG2	2.39	0.52
1:B:571:GLU:HA	1:B:571:GLU:OE1	2.10	0.52
1:B:482:LEU:HD23	1:B:492:ARG:NH1	2.24	0.52
1:B:666:TYR:CE2	3:B:1771:GVB:H12	2.45	0.52
1:A:115:LEU:CD2	1:A:132:TYR:CD1	2.92	0.52
1:B:116:LEU:O	1:B:132:TYR:HA	2.08	0.52
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.44	0.52
1:A:402:TRP:HA	4:A:2043:HOH:O	2.10	0.52
1:B:513:LYS:O	1:B:527:GLN:HA	2.10	0.52
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.92	0.52
1:A:372:TYR:CE1	1:A:410:LEU:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:LEU:HA	1:A:503:MET:HE3	1.91	0.52
1:B:164:LEU:HB2	1:B:175:LYS:HB2	1.92	0.51
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.46	0.51
1:B:163:LYS:HZ3	1:B:273:THR:HG23	1.73	0.51
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.93	0.51
1:B:713:PHE:O	1:B:714:GLN:C	2.54	0.51
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.92	0.51
1:A:644:SER:HB2	1:A:646:VAL:HG23	1.92	0.51
1:A:696:LYS:CG	1:A:697:GLN:HG3	2.41	0.51
1:A:88:VAL:HG12	1:A:88:VAL:O	2.10	0.51
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.46	0.51
1:B:51:ASN:OD1	1:B:54:ARG:HG3	2.10	0.51
1:B:401:THR:O	1:B:401:THR:HG22	2.11	0.51
1:B:316:LEU:HD22	1:B:359:PRO:HD3	1.93	0.51
1:A:74:ASN:CB	1:A:92:ASN:HB2	2.41	0.50
1:B:481:THR:CB	1:B:483:HIS:HE1	2.23	0.50
1:B:341:VAL:C	1:B:343:ARG:H	2.20	0.50
1:A:526:TYR:C	1:A:526:TYR:CD2	2.89	0.50
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.50
1:A:549:GLY:HA2	1:A:631:TYR:CE1	2.47	0.50
1:B:402:TRP:NE1	1:B:421:GLU:HG3	2.26	0.50
1:A:285:ILE:HD12	1:A:336:ARG:NH1	2.27	0.50
1:A:415:LEU:HD23	1:A:415:LEU:C	2.37	0.50
1:B:113:PHE:CE1	1:B:178:PRO:HG2	2.46	0.50
1:B:472:CYS:O	1:B:478:PRO:HA	2.12	0.50
1:B:258:LYS:NZ	1:B:712:HIS:ND1	2.60	0.50
1:A:219:ASN:ND2	1:A:221:THR:OG1	2.44	0.49
1:B:183:TYR:CD2	1:B:276:LEU:HB3	2.47	0.49
1:B:71:LYS:HA	1:B:75:ASN:O	2.11	0.49
1:B:311:ILE:HG22	1:B:312:SER:N	2.27	0.49
1:A:44:THR:O	1:A:47:ASP:HB2	2.12	0.49
1:A:739:ASP:C	1:A:739:ASP:OD1	2.55	0.49
1:B:110:ASP:CG	1:B:161:GLY:H	2.20	0.49
1:B:706:THR:HG1	1:B:737:ASP:H	1.60	0.49
1:B:134:ILE:HD13	1:B:178:PRO:CB	2.42	0.49
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.77	0.49
1:B:680:LEU:HD22	1:B:684:ARG:HD3	1.95	0.49
1:A:377:ASN:ND2	1:A:380:GLY:N	2.61	0.49
1:B:208:PHE:O	1:B:209:SER:C	2.54	0.49
1:A:635:VAL:O	1:A:639:VAL:HG23	2.12	0.48
1:B:201:TRP:CZ2	1:B:710:ASN:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:PRO:HG3	1:B:623:ARG:CZ	2.43	0.48
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.94	0.48
1:A:532:PRO:O	1:A:533:HIS:C	2.56	0.48
1:A:717:ALA:HB1	1:B:736:THR:CG2	2.42	0.48
1:A:730:PHE:O	1:B:733:MET:HE1	2.12	0.48
1:A:176:ILE:CD1	1:A:273:THR:HG22	2.43	0.48
1:A:221:THR:HG23	1:A:274:ASP:OD2	2.13	0.48
1:B:481:THR:HB	1:B:483:HIS:CE1	2.48	0.48
1:B:538:LYS:O	1:B:618:PHE:HA	2.13	0.48
1:B:594:ILE:HD11	1:B:602:GLU:H	1.78	0.48
1:B:635:VAL:O	1:B:636:THR:C	2.56	0.48
1:B:160:VAL:CG2	1:B:219:ASN:O	2.61	0.48
1:B:316:LEU:HD21	1:B:320:GLN:HG2	1.96	0.48
1:B:435:GLN:HE21	1:B:441:LYS:HB3	1.79	0.48
1:B:600:THR:HG21	4:B:2055:HOH:O	2.12	0.48
1:A:65:ASP:HB2	1:A:466:LYS:HG3	1.96	0.48
1:A:446:SER:HA	1:A:449:LEU:CD1	2.44	0.48
1:A:696:LYS:HG3	1:A:697:GLN:CG	2.43	0.48
1:B:148:ILE:HG23	1:B:149:PRO:HD2	1.96	0.48
1:A:217:SER:HB3	1:A:222:PHE:HB2	1.96	0.47
1:A:626:ILE:HG23	1:A:626:ILE:O	2.14	0.47
1:B:160:VAL:HG23	1:B:219:ASN:O	2.14	0.47
1:B:564:ALA:O	1:B:565:THR:C	2.56	0.47
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.49	0.47
1:A:602:GLU:OE1	1:A:602:GLU:N	2.48	0.47
1:A:109:PRO:HA	4:A:2006:HOH:O	2.13	0.47
1:A:708:ASP:OD2	1:A:740:HIS:HA	2.15	0.47
1:A:150:ASN:HD21	2:A:1767:NAG:H2	1.78	0.47
1:A:377:ASN:ND2	1:A:379:GLU:H	2.13	0.47
1:B:123:GLN:HB3	1:B:127:SER:OG	2.15	0.47
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.97	0.47
1:B:111:GLY:O	1:B:137:LEU:HD12	2.14	0.47
1:B:290:PRO:HD3	1:B:315:TRP:CD1	2.50	0.47
1:B:293:MET:O	1:B:298:HIS:CD2	2.68	0.47
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.49	0.47
1:A:657:SER:H	1:A:715:GLN:NE2	2.13	0.47
1:B:62:TRP:CG	1:B:462:SER:HA	2.50	0.47
1:B:293:MET:CE	1:B:324:VAL:HG23	2.43	0.47
1:A:219:ASN:N	1:A:308:GLN:OE1	2.48	0.46
1:B:658:ARG:HH22	1:B:684:ARG:NH2	2.11	0.46
1:A:630:SER:HB3	3:A:1771:GVB:C13	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:PRO:O	1:A:711:VAL:HG11	2.15	0.46
1:A:756:SER:O	1:A:760:LYS:CG	2.50	0.46
1:B:47:ASP:HA	1:B:52:THR:OG1	2.15	0.46
1:B:550:PRO:O	1:B:551:CYS:HB3	2.16	0.46
1:B:113:PHE:CD1	1:B:178:PRO:HG2	2.51	0.46
1:B:519:LEU:O	1:B:520:ASN:C	2.59	0.46
1:B:372:TYR:CE2	1:B:386:TYR:HD1	2.34	0.46
1:A:384:ILE:CG2	1:A:397:ILE:HD11	2.46	0.46
1:A:236:ILE:HG12	1:A:712:HIS:CD2	2.51	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.51	0.46
1:A:219:ASN:HB3	1:A:221:THR:H	1.81	0.46
1:A:355:GLY:HA3	1:A:358:ARG:O	2.15	0.46
1:A:382:ARG:H	1:A:403:GLU:HG2	1.81	0.46
1:B:109:PRO:HG2	1:B:158:SER:O	2.16	0.46
1:B:138:ASN:O	1:B:139:LYS:CG	2.64	0.46
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.99	0.45
1:B:382:ARG:HH21	1:B:591:MET:HE1	1.81	0.45
1:A:424:GLY:O	1:A:426:PRO:HD3	2.16	0.45
1:A:656:VAL:HG13	1:A:715:GLN:HE22	1.81	0.45
1:A:158:SER:OG	1:A:163:LYS:HB2	2.16	0.45
1:A:696:LYS:HE2	1:A:697:GLN:NE2	2.11	0.45
1:B:450:ASN:HB2	1:B:453:ARG:HB3	1.98	0.45
1:B:305:TRP:CH2	1:B:311:ILE:HD11	2.51	0.45
1:B:516:PHE:CD1	1:B:523:LYS:HG2	2.51	0.45
1:B:544:LEU:HD21	1:B:606:GLN:OE1	2.15	0.45
1:A:402:TRP:HB2	1:A:420:ASN:ND2	2.32	0.45
1:A:539:LYS:HE3	1:A:617:GLY:O	2.17	0.45
1:B:154:TRP:HD1	1:B:214:LEU:HD22	1.81	0.45
1:B:237:GLU:CG	1:B:253:ARG:HG2	2.42	0.45
1:B:517:ILE:HD12	1:B:519:LEU:CD1	2.46	0.45
1:B:543:LEU:HD12	1:B:567:LEU:HD13	1.98	0.45
1:A:246:LEU:CD1	1:A:248:TYR:O	2.65	0.45
1:A:603:VAL:O	1:A:605:ASP:N	2.50	0.45
1:A:105:TYR:CD1	1:A:105:TYR:C	2.95	0.45
1:A:326:ASP:OD2	1:A:339:CYS:CB	2.61	0.45
1:B:594:ILE:HD11	1:B:602:GLU:OE1	2.17	0.45
1:A:88:VAL:O	1:A:88:VAL:CG1	2.65	0.45
1:B:341:VAL:C	1:B:343:ARG:N	2.74	0.45
1:A:715:GLN:HB3	1:A:715:GLN:HE21	1.55	0.44
1:B:658:ARG:HG3	1:B:687:THR:HG22	1.99	0.44
1:A:258:LYS:HG2	1:A:661:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TRP:O	1:A:323:SER:HA	2.18	0.44
1:A:431:LEU:HD23	1:A:431:LEU:HA	1.68	0.44
1:A:526:TYR:HB3	1:A:578:PHE:HD1	1.82	0.44
1:A:549:GLY:HA2	1:A:631:TYR:CD1	2.52	0.44
1:B:299:TYR:CE2	1:B:318:ARG:HA	2.52	0.44
1:B:543:LEU:HD21	1:B:627:TRP:HD1	1.83	0.44
1:A:327:ILE:HB	1:A:343:ARG:HG3	2.00	0.44
1:A:541:PRO:HG2	1:A:573:ILE:HA	2.00	0.44
1:B:751:ILE:O	1:B:755:MET:HG3	2.17	0.44
1:A:435:GLN:HE21	1:A:441:LYS:HD3	1.83	0.44
1:B:46:THR:O	1:B:47:ASP:C	2.59	0.44
1:B:327:ILE:HD13	1:B:389:ILE:HG12	2.00	0.44
1:A:76:ILE:HD12	1:A:90:LEU:HD12	1.99	0.44
1:A:553:GLN:HA	1:A:579:ASP:OD2	2.18	0.44
1:A:623:ARG:HD3	1:A:763:PHE:O	2.17	0.44
1:B:402:TRP:CE2	1:B:421:GLU:HG3	2.53	0.44
1:B:535:ASP:OD2	1:B:538:LYS:HG3	2.17	0.44
1:B:626:ILE:O	1:B:650:GLY:HA2	2.18	0.43
1:A:417:TYR:HE2	1:A:419:SER:HB3	1.82	0.43
1:A:420:ASN:C	1:A:420:ASN:HD22	2.26	0.43
1:B:82:GLU:HG3	1:B:83:TYR:CD2	2.53	0.43
1:B:543:LEU:HD12	1:B:567:LEU:CD1	2.48	0.43
1:A:167:VAL:HG21	1:A:198:ILE:HG23	2.00	0.43
1:B:225:TYR:CZ	1:B:269:PHE:HB2	2.53	0.43
1:A:377:ASN:ND2	1:A:379:GLU:N	2.66	0.43
1:A:446:SER:O	1:A:447:CYS:C	2.60	0.43
1:A:601:PHE:O	1:A:602:GLU:C	2.62	0.43
1:B:135:TYR:HD2	1:B:142:LEU:HD23	1.84	0.43
1:B:658:ARG:NH2	1:B:684:ARG:HH21	2.16	0.43
1:A:246:LEU:HD11	1:A:248:TYR:O	2.19	0.43
1:A:736:THR:HG21	1:B:717:ALA:O	2.18	0.43
1:B:623:ARG:NH1	1:B:763:PHE:O	2.50	0.43
1:A:471:ARG:HB2	1:A:480:TYR:CD2	2.54	0.43
1:B:600:THR:CG2	1:B:601:PHE:N	2.71	0.43
1:A:377:ASN:ND2	1:A:380:GLY:H	2.17	0.43
1:A:603:VAL:O	1:A:604:GLU:C	2.62	0.43
1:A:636:THR:HG21	1:A:651:ILE:O	2.18	0.43
1:A:760:LYS:HB3	1:A:760:LYS:HE3	1.67	0.43
1:B:138:ASN:C	1:B:139:LYS:CG	2.91	0.43
1:B:183:TYR:N	1:B:183:TYR:CD1	2.87	0.43
1:B:694:ASN:C	1:B:696:LYS:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD21	1:A:132:TYR:CD1	2.53	0.43
1:B:61:ARG:O	1:B:63:ILE:HD13	2.19	0.43
1:A:116:LEU:O	1:A:132:TYR:HA	2.19	0.43
1:A:360:SER:OG	1:A:373:LYS:HG3	2.18	0.43
1:B:314:GLN:NE2	1:B:362:PRO:HD3	2.34	0.43
1:B:382:ARG:NH2	1:B:591:MET:HE1	2.34	0.43
1:B:696:LYS:HG3	1:B:728:VAL:HG22	2.00	0.43
1:A:365:THR:CG2	1:A:372:TYR:HE1	2.31	0.43
1:A:377:ASN:HD21	1:A:380:GLY:N	2.16	0.43
1:A:529:ILE:O	1:A:529:ILE:HG22	2.17	0.43
1:A:666:TYR:O	1:A:670:TYR:CD2	2.72	0.43
1:A:154:TRP:O	1:A:166:TYR:HA	2.19	0.42
1:A:597:ARG:HA	1:A:682:HIS:CD2	2.54	0.42
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.18	0.42
1:B:405:ILE:HG12	1:B:429:ARG:CZ	2.48	0.42
1:A:74:ASN:HB2	1:A:92:ASN:CB	2.49	0.42
1:A:397:ILE:HG13	1:A:398:THR:HG23	2.01	0.42
1:B:68:TYR:CD1	1:B:68:TYR:C	2.97	0.42
1:A:65:ASP:HA	1:A:463:LYS:O	2.19	0.42
1:A:153:GLN:HE22	1:A:170:ASN:H	1.67	0.42
1:A:666:TYR:CE2	3:A:1771:GVB:H19	2.53	0.42
1:B:417:TYR:CE1	1:B:434:ILE:HD11	2.54	0.42
1:B:481:THR:CB	1:B:483:HIS:CE1	3.02	0.42
1:A:666:TYR:CD2	3:A:1771:GVB:H19	2.55	0.42
1:B:271:VAL:HG22	1:B:284:SER:HA	2.02	0.42
1:B:305:TRP:CE3	1:B:311:ILE:HG12	2.55	0.42
1:A:542:LEU:HA	1:A:574:ILE:O	2.19	0.42
1:B:582:GLY:HA2	1:B:591:MET:O	2.19	0.42
1:B:237:GLU:HA	1:B:252:VAL:O	2.19	0.42
1:B:579:ASP:HB2	4:B:2048:HOH:O	2.20	0.42
1:A:631:TYR:O	1:A:635:VAL:HG23	2.20	0.42
1:B:134:ILE:HB	1:B:143:ILE:HG12	2.01	0.42
1:B:450:ASN:N	1:B:450:ASN:ND2	2.68	0.42
1:A:499:ALA:HA	1:A:502:LYS:HD3	2.02	0.41
1:B:167:VAL:HG11	1:B:198:ILE:HD13	2.02	0.41
1:B:377:ASN:C	1:B:377:ASN:ND2	2.77	0.41
1:B:678:ASP:HB3	1:B:679:ASN:H	1.63	0.41
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.85	0.41
1:B:543:LEU:HD21	1:B:627:TRP:CD1	2.55	0.41
1:B:749:GLN:O	1:B:753:THR:OG1	2.37	0.41
1:A:453:ARG:NH2	1:A:496:ASP:O	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:CYS:HB3	1:B:457:TYR:CZ	2.55	0.41
1:B:454:CYS:HB3	1:B:457:TYR:CE2	2.55	0.41
1:A:55:LEU:HD22	1:A:478:PRO:HG2	2.02	0.41
1:A:208:PHE:O	1:A:209:SER:C	2.62	0.41
1:A:633:GLY:C	1:A:655:PRO:HB3	2.46	0.41
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.49	0.41
1:A:475:PRO:O	1:A:559:PHE:HB2	2.21	0.41
1:A:626:ILE:HB	1:A:647:PHE:CE2	2.55	0.41
1:B:689:MET:C	1:B:691:ARG:H	2.29	0.41
1:A:143:ILE:HG21	1:A:179:ASN:CB	2.50	0.41
1:A:369:ASN:HA	1:A:389:ILE:HD12	2.02	0.41
1:A:754:HIS:ND1	1:B:729:ASP:OD1	2.34	0.41
1:B:169:ASN:O	1:B:170:ASN:HB2	2.20	0.41
1:B:382:ARG:HG3	1:B:403:GLU:CD	2.46	0.41
1:B:571:GLU:CD	1:B:760:LYS:HD3	2.46	0.41
1:A:163:LYS:NZ	1:A:274:ASP:OD1	2.54	0.41
1:A:301:CYS:SG	1:A:359:PRO:HG2	2.61	0.41
1:A:304:THR:O	1:A:312:SER:HB3	2.21	0.41
1:A:109:PRO:HG2	1:A:158:SER:O	2.20	0.41
1:A:384:ILE:HG13	1:A:404:VAL:HG21	2.03	0.41
1:A:403:GLU:OE2	1:A:587:GLY:HA2	2.20	0.41
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.84	0.41
1:B:65:ASP:OD1	1:B:65:ASP:N	2.49	0.41
1:B:306:ALA:HB3	1:B:310:ARG:HG2	2.03	0.41
1:B:626:ILE:HG23	1:B:636:THR:HG23	2.03	0.41
1:B:643:GLY:C	1:B:645:GLY:N	2.78	0.41
1:A:184:ARG:HG2	1:A:186:THR:O	2.20	0.41
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.21	0.41
1:B:69:LEU:HD13	1:B:107:ILE:HD12	2.02	0.41
1:A:471:ARG:O	1:A:471:ARG:HG3	2.21	0.40
1:B:571:GLU:OE2	1:B:760:LYS:HD3	2.20	0.40
1:A:363:HIS:CE1	1:A:407:ILE:HB	2.57	0.40
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.85	0.40
1:B:310:ARG:NE	1:B:329:ASP:OD1	2.49	0.40
1:B:500:LEU:HA	1:B:503:MET:HE3	2.03	0.40
1:B:695:PHE:HA	1:B:698:VAL:HG22	2.03	0.40
1:B:644:SER:O	1:B:645:GLY:C	2.65	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	726/736 (99%)	639 (88%)	78 (11%)	9 (1%)	10	34
1	B	726/736 (99%)	637 (88%)	79 (11%)	10 (1%)	9	30
All	All	1452/1472 (99%)	1276 (88%)	157 (11%)	19 (1%)	9	31

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	486	VAL
1	A	73	GLU
1	A	604	GLU
1	B	94	THR
1	B	342	ALA
1	B	551	CYS
1	B	140	ARG
1	B	320	GLN
1	B	725	ASP
1	A	603	VAL
1	B	714	GLN
1	A	64	SER
1	A	111	GLY
1	A	588	ASP
1	B	244	GLU
1	B	615	LYS
1	B	742	ILE
1	A	359	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	653/658 (99%)	567 (87%)	86 (13%)	4	14
1	B	653/658 (99%)	573 (88%)	80 (12%)	4	16
All	All	1306/1316 (99%)	1140 (87%)	166 (13%)	4	15

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	44	THR
1	A	49	LEU
1	A	60	LEU
1	A	88	VAL
1	A	90	LEU
1	A	91	GLU
1	A	94	THR
1	A	102	ILE
1	A	115	LEU
1	A	122	LYS
1	A	140	ARG
1	A	141	GLN
1	A	142	LEU
1	A	143	ILE
1	A	144	THR
1	A	158	SER
1	A	160	VAL
1	A	178	PRO
1	A	180	LEU
1	A	182	SER
1	A	202	VAL
1	A	212	SER
1	A	223	LEU
1	A	230	ASP
1	A	244	GLU
1	A	246	LEU
1	A	250	LYS
1	A	251	THR
1	A	254	VAL
1	A	284	SER
1	A	294	LEU
1	A	311	ILE

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Mol	Chain	Res	Type
1	A	316	LEU
1	A	326	ASP
1	A	341	VAL
1	A	343	ARG
1	A	348	MET
1	A	366	LEU
1	A	373	LYS
1	A	377	ASN
1	A	379	GLU
1	A	393	ASP
1	A	405	ILE
1	A	410	LEU
1	A	418	ILE
1	A	419	SER
1	A	420	ASN
1	A	425	MET
1	A	431	LEU
1	A	434	ILE
1	A	442	VAL
1	A	443	THR
1	A	455	GLN
1	A	458	SER
1	A	462	SER
1	A	471	ARG
1	A	479	LEU
1	A	481	THR
1	A	482	LEU
1	A	485	SER
1	A	486	VAL
1	A	487	ASN
1	A	500	LEU
1	A	505	GLN
1	A	513	LYS
1	A	514	LEU
1	A	515	ASP
1	A	519	LEU
1	A	521	GLU
1	A	522	THR
1	A	523	LYS
1	A	543	LEU
1	A	544	LEU
1	A	594	ILE

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Mol	Chain	Res	Type
1	A	608	GLU
1	A	621	ASN
1	A	636	THR
1	A	646	VAL
1	A	673	LEU
1	A	677	GLU
1	A	684	ARG
1	A	715	GLN
1	A	736	THR
1	A	745	SER
1	A	760	LYS
1	B	41	LYS
1	B	46	THR
1	B	49	LEU
1	B	50	LYS
1	B	60	LEU
1	B	63	ILE
1	B	86	SER
1	B	90	LEU
1	B	91	GLU
1	B	93	SER
1	B	94	THR
1	B	96	ASP
1	B	114	ILE
1	B	120	TYR
1	B	129	THR
1	B	151	ASN
1	B	152	THR
1	B	155	VAL
1	B	156	THR
1	B	160	VAL
1	B	180	LEU
1	B	183	TYR
1	B	194	ILE
1	B	198	ILE
1	B	202	VAL
1	B	214	LEU
1	B	223	LEU
1	B	236	ILE
1	B	246	LEU
1	B	247	GLN
1	B	263	ASN

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Mol	Chain	Res	Type
1	B	267	LYS
1	B	278	SER
1	B	280	THR
1	B	283	THR
1	B	285	ILE
1	B	288	THR
1	B	295	ILE
1	B	300	LEU
1	B	326	ASP
1	B	339	CYS
1	B	340	LEU
1	B	350	THR
1	B	365	THR
1	B	366	LEU
1	B	373	LYS
1	B	377	ASN
1	B	385	CYS
1	B	388	GLN
1	B	389	ILE
1	B	392	LYS
1	B	399	LYS
1	B	401	THR
1	B	412	SER
1	B	420	ASN
1	B	435	GLN
1	B	450	ASN
1	B	472	CYS
1	B	479	LEU
1	B	486	VAL
1	B	500	LEU
1	B	514	LEU
1	B	517	ILE
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	570	THR
1	B	590	ILE
1	B	594	ILE
1	B	619	VAL
1	B	620	ASP
1	B	621	ASN
1	B	624	ILE

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Mol	Chain	Res	Type
1	B	630	SER
1	B	663	ASP
1	B	680	LEU
1	B	715	GLN
1	B	726	VAL
1	B	736	THR
1	B	764	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	103	ASN
1	A	123	GLN
1	A	141	GLN
1	A	153	GLN
1	A	219	ASN
1	A	227	GLN
1	A	281	ASN
1	A	298	HIS
1	A	377	ASN
1	A	420	ASN
1	A	435	GLN
1	A	450	ASN
1	A	487	ASN
1	A	508	GLN
1	A	533	HIS
1	A	621	ASN
1	A	679	ASN
1	A	697	GLN
1	A	715	GLN
1	A	748	HIS
1	B	103	ASN
1	B	151	ASN
1	B	169	ASN
1	B	229	ASN
1	B	247	GLN
1	B	263	ASN
1	B	286	GLN
1	B	298	HIS
1	B	314	GLN
1	B	363	HIS

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Mol	Chain	Res	Type
1	B	377	ASN
1	B	383	HIS
1	B	388	GLN
1	B	420	ASN
1	B	435	GLN
1	B	450	ASN
1	B	483	HIS
1	B	562	ASN
1	B	572	ASN
1	B	586	GLN
1	B	621	ASN
1	B	679	ASN
1	B	715	GLN
1	B	750	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	NAG	B	1767	1	14,14,15	0.62	0	17,19,21	1.84	4 (23%)
2	NAG	A	1769	-	14,14,15	0.54	0	17,19,21	0.91	1 (5%)
3	GVB	A	1771	-	26,26,26	0.63	0	33,36,36	1.01	2 (6%)
2	NAG	B	1770	1	14,14,15	0.80	1 (7%)	17,19,21	1.52	3 (17%)
2	NAG	A	1770	1	14,14,15	0.54	0	17,19,21	1.55	2 (11%)
2	NAG	A	1767	-	14,14,15	0.62	0	17,19,21	1.88	6 (35%)
2	NAG	A	1768	-	14,14,15	0.62	0	17,19,21	1.29	2 (11%)
2	NAG	B	1769	-	14,14,15	0.90	0	17,19,21	1.75	5 (29%)
2	NAG	B	1768	1	14,14,15	0.61	0	17,19,21	1.40	3 (17%)
3	GVB	B	1771	-	26,26,26	0.60	0	33,36,36	1.09	2 (6%)

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	NAG	B	1767	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1769	-	-	2/6/23/26	0/1/1/1
3	GVB	A	1771	-	-	0/12/25/25	0/3/3/3
2	NAG	B	1770	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	1770	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1767	-	-	5/6/23/26	0/1/1/1
2	NAG	A	1768	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1769	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1768	1	-	2/6/23/26	0/1/1/1
3	GVB	B	1771	-	-	0/12/25/25	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1770	NAG	C1-C2	2.58	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1770	NAG	C1-O5-C5	4.66	118.44	112.19
2	B	1767	NAG	C1-O5-C5	4.36	118.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1767	NAG	O5-C1-C2	-4.21	104.77	111.29
2	A	1768	NAG	O5-C1-C2	-3.35	106.11	111.29
2	A	1767	NAG	C3-C4-C5	3.35	116.30	110.23
2	B	1770	NAG	O5-C5-C6	3.32	114.11	107.66
2	B	1767	NAG	C1-C2-N2	3.31	115.65	110.43
2	B	1769	NAG	C2-N2-C7	-3.30	118.48	122.90
2	B	1767	NAG	C2-N2-C7	3.25	127.26	122.90
2	B	1770	NAG	C3-C4-C5	-3.17	104.49	110.23
2	B	1769	NAG	O5-C1-C2	-3.07	106.55	111.29
2	B	1769	NAG	C1-C2-N2	-3.00	105.70	110.43
2	A	1767	NAG	O5-C5-C4	2.84	117.73	110.83
2	B	1770	NAG	O5-C1-C2	2.56	115.25	111.29
3	A	1771	GVB	O26-C6-C5	2.48	118.76	115.40
2	A	1767	NAG	C1-O5-C5	2.38	115.38	112.19
2	A	1767	NAG	C2-N2-C7	2.37	126.08	122.90
2	B	1768	NAG	O3-C3-C4	-2.37	104.79	110.38
3	B	1771	GVB	O25-C5-C6	2.35	118.58	115.40
3	B	1771	GVB	O26-C6-C5	2.32	118.56	115.40
2	B	1768	NAG	O5-C1-C2	-2.26	107.79	111.29
2	A	1767	NAG	C4-C3-C2	-2.22	107.77	111.02
2	A	1769	NAG	O5-C1-C2	-2.21	107.88	111.29
2	B	1769	NAG	O6-C6-C5	-2.19	103.87	111.33
3	A	1771	GVB	O25-C5-C6	2.19	118.37	115.40
2	A	1768	NAG	C1-O5-C5	-2.18	109.27	112.19
2	B	1768	NAG	C1-O5-C5	2.16	115.08	112.19
2	B	1769	NAG	C6-C5-C4	2.12	118.22	113.02
2	A	1770	NAG	C3-C4-C5	-2.10	106.43	110.23
2	B	1767	NAG	O5-C1-C2	-2.02	108.17	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1770	NAG	C1

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1767	NAG	C3-C2-N2-C7
2	A	1767	NAG	C8-C7-N2-C2
2	A	1767	NAG	O7-C7-N2-C2
2	B	1767	NAG	C1-C2-N2-C7
2	B	1767	NAG	C8-C7-N2-C2

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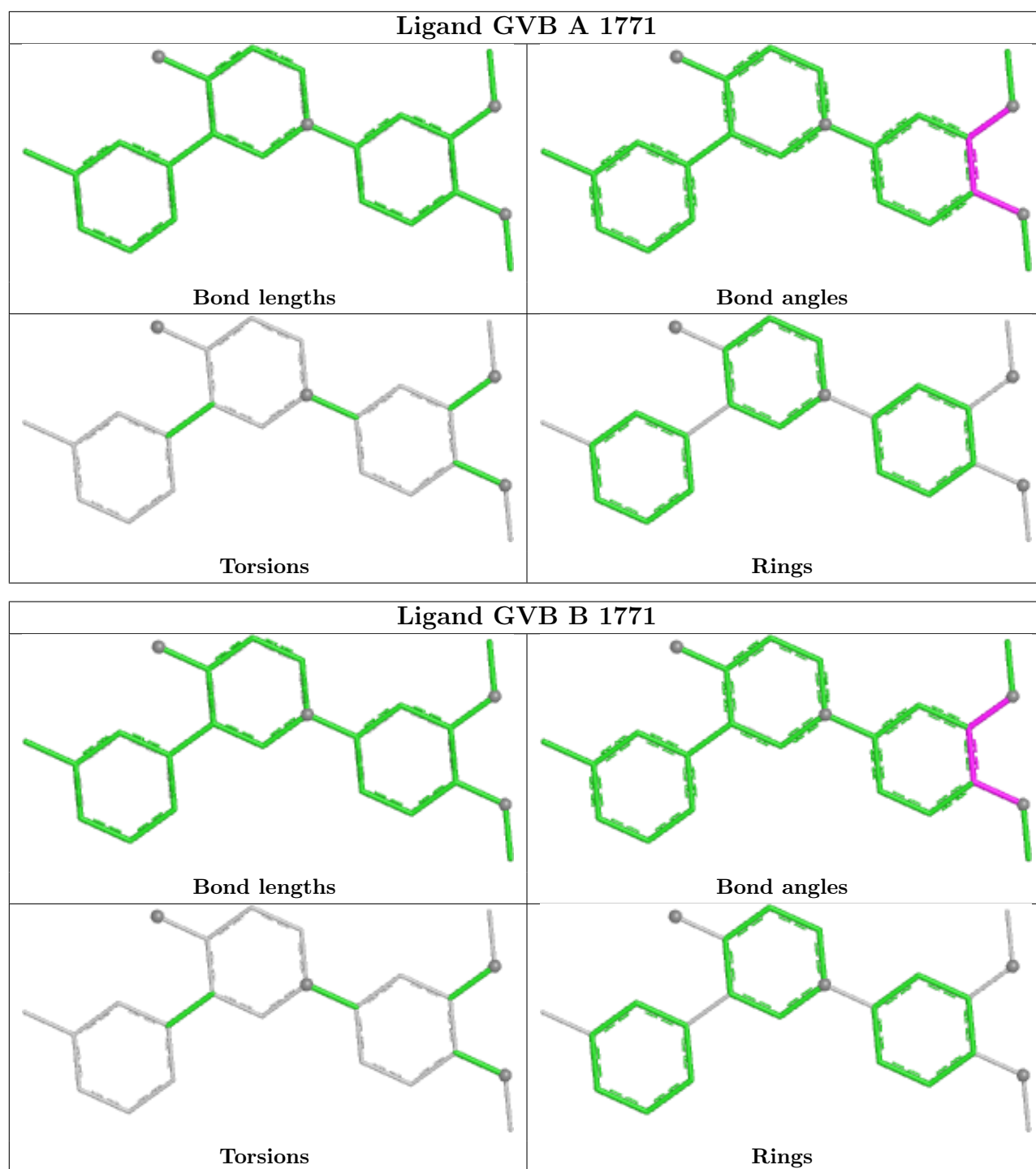
Mol	Chain	Res	Type	Atoms
2	B	1767	NAG	O7-C7-N2-C2
2	B	1770	NAG	C8-C7-N2-C2
2	B	1770	NAG	O7-C7-N2-C2
2	A	1769	NAG	O7-C7-N2-C2
2	B	1770	NAG	O5-C5-C6-O6
2	A	1770	NAG	O5-C5-C6-O6
2	A	1768	NAG	O5-C5-C6-O6
2	A	1769	NAG	C8-C7-N2-C2
2	B	1768	NAG	C8-C7-N2-C2
2	B	1770	NAG	C4-C5-C6-O6
2	A	1768	NAG	C4-C5-C6-O6
2	B	1768	NAG	O7-C7-N2-C2
2	A	1770	NAG	C4-C5-C6-O6
2	A	1767	NAG	C4-C5-C6-O6
2	A	1767	NAG	O5-C5-C6-O6
2	A	1770	NAG	C8-C7-N2-C2
2	A	1770	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1769	NAG	2	0
3	A	1771	GVB	3	0
2	A	1767	NAG	4	0
2	A	1768	NAG	4	0
2	B	1769	NAG	3	0
3	B	1771	GVB	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.