



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 07:20 pm BST

PDB ID : 2JID
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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

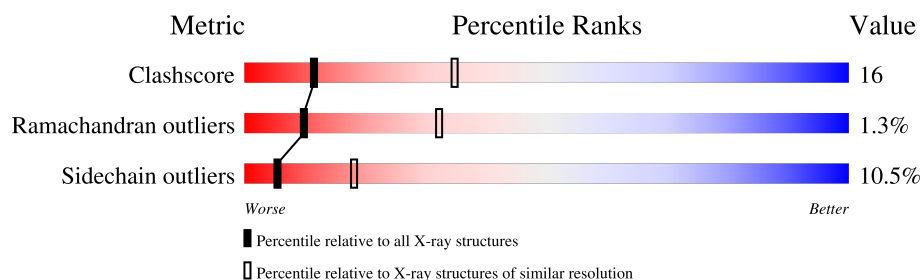
1 Overall quality at a glance

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	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



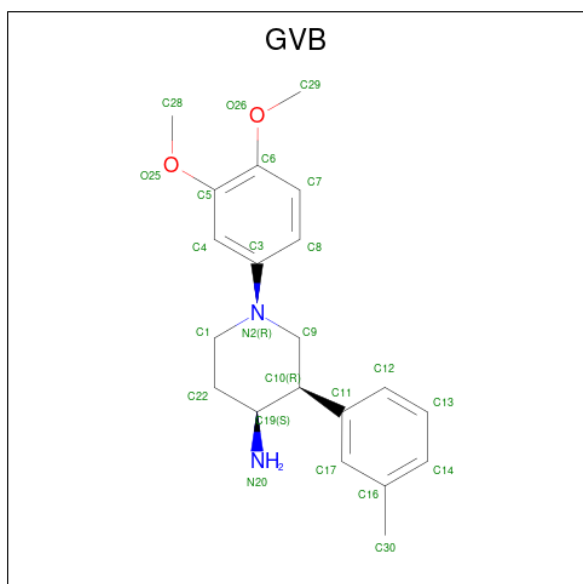
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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 (three-letter code: 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.

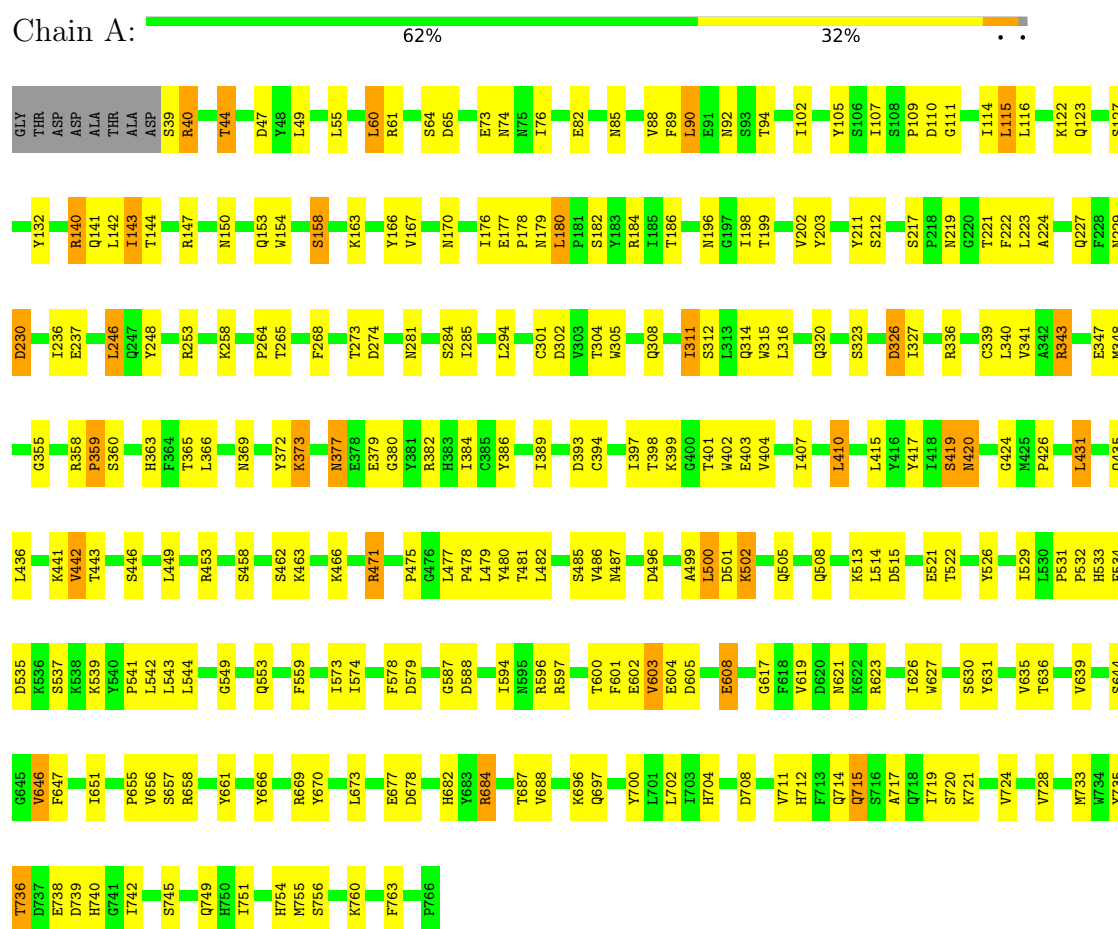
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	73	Total	O	0	0
			73	73		

3 Residue-property plots

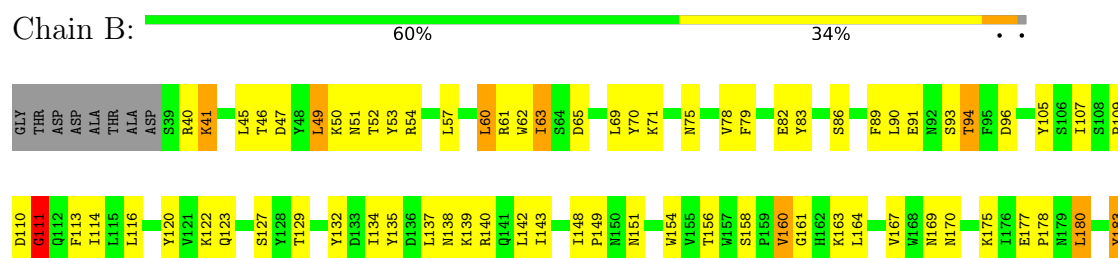
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



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V698	G599	R492	E378	V779	I193
S699	T600	L500	E379	T280	I194
Y700	F601	N506	G380	T283	Y195
N710	V603	M509	Y381	S284	I198
V711	Q606	P510	C385	T288	W201
H712	R611	K513	Y386	A289	V202
F713	S614	L514	F387	P290	F208
Q714	K615	D515	Q388	M293	S209
W715	F618	F516	I389	L294	S209
S716	V619	I517	K392	I295	L214
A717	D620	I518	K399	H298	L214
A717	N621	L519	G400	Y299	N219
D725	W622	N520	T401	L300	G220
V726	R623	K523	W402	G301	T221
V727	I624	Q527	E403	D302	F222
G727	A625	D535	W404	W305	L223
V728	W626	K538	I405	A306	A224
V729	I627	P541	S412	R310	A226
D729	S630	L542	Y414	I311	Q227
Y735	V635	L544	L415	S312	F228
T736	K648	P550	Y416	L313	N229
T736	G649	C551	Y417	Q314	P234
G741	G650	V558	K441	W315	L235
I742	S657	N562	N450	L316	L236
Q749	R658	W563	R453	R317	E237
H750	D663	A564	C454	R318	S242
I751	Y666	T565	Y457	I319	D243
Y752	R669	Y566	S462	Q320	E244
T753	T675	L567	E464	V324	S245
H754	D678	E571	E464	M325	L246
N755	N679	F578	L470	D326	Q247
K760	L680	D579	R471	I327	Y248
Q761	D681	G582	C472	C328	P249
C762	H682	Y585	P478	D329	V252
F763	Y683	M591	L479	L340	R253
S764	R684	H592	Y480	V341	K258
L765	T687	A593	T481	A342	N263
P766	F695	I594	L482	R343	V266
	K696	L598	H483	T350	K267
	Q697			T351	F268
				P359	F269
				P362	V271
				T365	N272
				Y372	T273
				K373	L276
				N377	S277
					S278

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	0.65	0/6135	0.77	3/8344 (0.0%)
1	B	0.68	1/6135 (0.0%)	0.78	4/8344 (0.0%)
All	All	0.67	1/12270 (0.0%)	0.78	7/16688 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	GLU	CG-CD	5.10	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	LEU	CA-CB-CG	6.71	130.72	115.30
1	A	60	LEU	CA-CB-CG	6.30	129.79	115.30
1	A	500	LEU	CA-CB-CG	6.21	129.59	115.30
1	B	111	GLY	N-CA-C	5.43	126.68	113.10
1	B	57	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	442	VAL	CB-CA-C	-5.25	101.42	111.40
1	B	253	ARG	NE-CZ-NH1	5.25	122.92	120.30

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 ⓘ

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	196	0
1	B	5963	0	5681	186	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	5	0
4	A	55	0	0	5	0
4	B	73	0	0	4	0
All	All	12214	0	11521	373	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 16.

All (373) 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:B:597:ARG:O	1:B:600:THR:HG22	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:377:ASN:C	1:A:377:ASN:HD22	1.93	0.72
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:ASN:C	1:A:92:ASN:HB3	2.18	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: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:630:SER:HB3	3:B:1771:GVB:H302	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:751:ILE:HG12	1:A:755:MET:CE	2.32	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:A:657:SER:OG	1:A:715:GLN:HB3	2.03	0.58
1:A:721:LYS:NZ	1:B:242:SER:O	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:VAL:CG2	3:B:1771:GVB:H303	2.34	0.58
1:A:340:LEU:HB2	1:A:343:ARG:HD3	1.86	0.58
1:B:377:ASN:C	1:B:377:ASN:HD22	2.07	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:377:ASN:C	1:A:377:ASN:ND2	2.59	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: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:B:138:ASN:C	1:B:139:LYS:HG3	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:302:ASP:HB3	1:A:314:GLN:HB2	1.93	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:562:ASN:C	1:B:562:ASN:HD22	2.14	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: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:711:VAL:HG23	3:B:1771:GVB:H303	1.93	0.50
1:A:735:TYR:O	1:A:736:THR:C	2.49	0.50
1:B:258:LYS:NZ	1:B:712:HIS:ND1	2.60	0.50
1:B:637:SER:HG	1:B:700:TYR:HH	1.58	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:B:163:LYS:HZ3	1:B:273:THR:HG23	1.75	0.49
1:A:44:THR:O	1:A:47:ASP:HB2	2.12	0.49
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.95	0.49
1:B:134:ILE:HD13	1:B:178:PRO:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:293:MET:CE	1:B:324:VAL:HG23	2.43	0.48
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:717:ALA:HB1	1:B:736:THR:CG2	2.42	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: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: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: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:713:PHE:O	1:B:714:GLN:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:SER:HB3	3:A:1771:GVB:C13	2.44	0.46
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: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:341:VAL:C	1:B:343:ARG:H	2.20	0.46
1:A:526:TYR:CD2	1:A:526:TYR:C	2.89	0.46
1:B:138:ASN:O	1:B:139:LYS:CG	2.64	0.46
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.46
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.99	0.45
1:A:424:GLY:O	1:A:426:PRO:HD3	2.16	0.45
1:A:415:LEU:HD23	1:A:415:LEU:C	2.37	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:208:PHE:O	1:B:209:SER:C	2.54	0.45
1:B:450:ASN:HB2	1:B:453:ARG:HB3	1.98	0.45
1:A:739:ASP:C	1:A:739:ASP:OD1	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:315:TRP:O	1:A:323:SER:HA	2.18	0.44
1:B:110:ASP:CG	1:B:161:GLY:H	2.20	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: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:A:532:PRO:O	1:A:533:HIS:C	2.56	0.43
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: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:B:135:TYR:HD2	1:B:142:LEU:HD23	1.84	0.43
1:B:635:VAL:O	1:B:636:THR:C	2.56	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: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:183:TYR:N	1:B:183:TYR:CD1	2.87	0.43
1:A:115:LEU:HD21	1:A:132:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ARG:O	1:B:63:ILE:HD13	2.19	0.43
1:B:564:ALA:O	1:B:565:THR:C	2.56	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: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:597:ARG:O	1:A:600:THR:OG1	2.25	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:293:MET:HE2	1:B:324:VAL:HG23	2.01	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: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:A:733:MET:HB2	1:A:733:MET:HE2	1.90	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: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:B:519:LEU:O	1:B:520:ASN:C	2.59	0.41
1:A:55:LEU:HD22	1:A:478:PRO:HG2	2.02	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: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: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: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:695:PHE:HA	1:B:698:VAL:HG22	2.03	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%)	11	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%)	10	32

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 ⓘ

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%)	584 (89%)	69 (11%)	5	18
1	B	653/658 (99%)	585 (90%)	68 (10%)	5	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1306/1316 (99%)	1169 (90%)	137 (10%)	5 18

All (137) 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	90	LEU
1	A	94	THR
1	A	102	ILE
1	A	115	LEU
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	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	246	LEU
1	A	284	SER
1	A	294	LEU
1	A	311	ILE
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	393	ASP
1	A	399	LYS
1	A	410	LEU
1	A	419	SER

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Mol	Chain	Res	Type
1	A	420	ASN
1	A	431	LEU
1	A	442	VAL
1	A	443	THR
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	487	ASN
1	A	500	LEU
1	A	502	LYS
1	A	505	GLN
1	A	513	LYS
1	A	514	LEU
1	A	515	ASP
1	A	521	GLU
1	A	522	THR
1	A	543	LEU
1	A	544	LEU
1	A	608	GLU
1	A	621	ASN
1	A	627	TRP
1	A	646	VAL
1	A	673	LEU
1	A	677	GLU
1	A	684	ARG
1	A	704	HIS
1	A	715	GLN
1	A	736	THR
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

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Mol	Chain	Res	Type
1	B	94	THR
1	B	96	ASP
1	B	120	TYR
1	B	129	THR
1	B	151	ASN
1	B	156	THR
1	B	160	VAL
1	B	180	LEU
1	B	183	TYR
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	263	ASN
1	B	267	LYS
1	B	278	SER
1	B	280	THR
1	B	283	THR
1	B	288	THR
1	B	295	ILE
1	B	299	TYR
1	B	300	LEU
1	B	326	ASP
1	B	340	LEU
1	B	350	THR
1	B	365	THR
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	450	ASN
1	B	472	CYS
1	B	479	LEU
1	B	500	LEU

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Mol	Chain	Res	Type
1	B	514	LEU
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	566	TYR
1	B	620	ASP
1	B	621	ASN
1	B	630	SER
1	B	663	ASP
1	B	679	ASN
1	B	680	LEU
1	B	684	ARG
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 (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	123	GLN
1	A	141	GLN
1	A	219	ASN
1	A	247	GLN
1	A	263	ASN
1	A	281	ASN
1	A	298	HIS
1	A	363	HIS
1	A	377	ASN
1	A	420	ASN
1	A	435	GLN
1	A	487	ASN
1	A	508	GLN
1	A	533	HIS
1	A	586	GLN
1	A	621	ASN
1	A	679	ASN
1	A	697	GLN
1	A	715	GLN
1	B	123	GLN
1	B	169	ASN

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Mol	Chain	Res	Type
1	B	229	ASN
1	B	247	GLN
1	B	263	ASN
1	B	286	GLN
1	B	298	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	435	GLN
1	B	450	ASN
1	B	483	HIS
1	B	562	ASN
1	B	621	ASN
1	B	679	ASN
1	B	682	HIS
1	B	694	ASN
1	B	715	GLN
1	B	731	GLN
1	B	750	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	1767	-	14,14,15	0.64	0	17,19,21	1.86	6 (35%)
2	NAG	A	1770	1	14,14,15	0.53	0	17,19,21	1.58	3 (17%)
2	NAG	B	1769	-	14,14,15	0.92	0	17,19,21	1.70	5 (29%)
2	NAG	A	1769	-	14,14,15	0.56	0	17,19,21	0.92	1 (5%)
2	NAG	B	1768	1	14,14,15	0.62	0	17,19,21	1.41	3 (17%)
3	GVB	A	1771	-	26,26,26	0.62	0	34,36,36	0.98	2 (5%)
3	GVB	B	1771	-	26,26,26	0.59	0	34,36,36	1.06	2 (5%)
2	NAG	B	1767	1	14,14,15	0.61	0	17,19,21	1.78	3 (17%)
2	NAG	B	1770	1	14,14,15	0.75	1 (7%)	17,19,21	1.67	3 (17%)
2	NAG	A	1768	-	14,14,15	0.65	0	17,19,21	1.31	2 (11%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1770	NAG	C1-C2	2.36	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	4.61	118.44	112.19
2	B	1770	NAG	O5-C5-C6	4.41	114.11	107.20
2	B	1767	NAG	C1-O5-C5	4.31	118.03	112.19
2	A	1767	NAG	O5-C1-C2	-4.13	104.77	111.29
2	A	1767	NAG	C3-C4-C5	3.40	116.30	110.24
2	A	1768	NAG	O5-C1-C2	-3.28	106.11	111.29
2	B	1770	NAG	C3-C4-C5	-3.22	104.49	110.24
2	B	1769	NAG	C2-N2-C7	-3.11	118.48	122.90
2	B	1767	NAG	C2-N2-C7	3.06	127.26	122.90
2	B	1767	NAG	C1-C2-N2	3.02	115.65	110.49
2	B	1769	NAG	O5-C1-C2	-3.00	106.55	111.29
2	A	1767	NAG	O5-C5-C4	2.84	117.73	110.83
2	B	1769	NAG	C1-C2-N2	-2.80	105.70	110.49
2	B	1770	NAG	O5-C1-C2	2.51	115.25	111.29
3	A	1771	GVB	O26-C6-C5	2.41	118.76	115.41
2	B	1768	NAG	O3-C3-C4	-2.40	104.79	110.35
2	A	1767	NAG	C1-O5-C5	2.35	115.38	112.19
3	B	1771	GVB	O25-C5-C6	2.28	118.58	115.41
3	B	1771	GVB	O26-C6-C5	2.26	118.56	115.41
2	A	1767	NAG	C2-N2-C7	2.23	126.08	122.90
2	B	1769	NAG	C6-C5-C4	2.23	118.22	113.00
2	A	1767	NAG	C4-C3-C2	-2.22	107.77	111.02
2	B	1768	NAG	O5-C1-C2	-2.22	107.79	111.29
2	B	1769	NAG	O6-C6-C5	-2.16	103.87	111.29
2	A	1769	NAG	O5-C1-C2	-2.16	107.88	111.29
2	A	1768	NAG	C1-O5-C5	-2.16	109.27	112.19
2	A	1770	NAG	C3-C4-C5	-2.14	106.43	110.24
2	B	1768	NAG	C1-O5-C5	2.14	115.08	112.19
3	A	1771	GVB	O25-C5-C6	2.13	118.37	115.41
2	A	1770	NAG	O5-C5-C6	2.09	110.48	107.20

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	C8-C7-N2-C2

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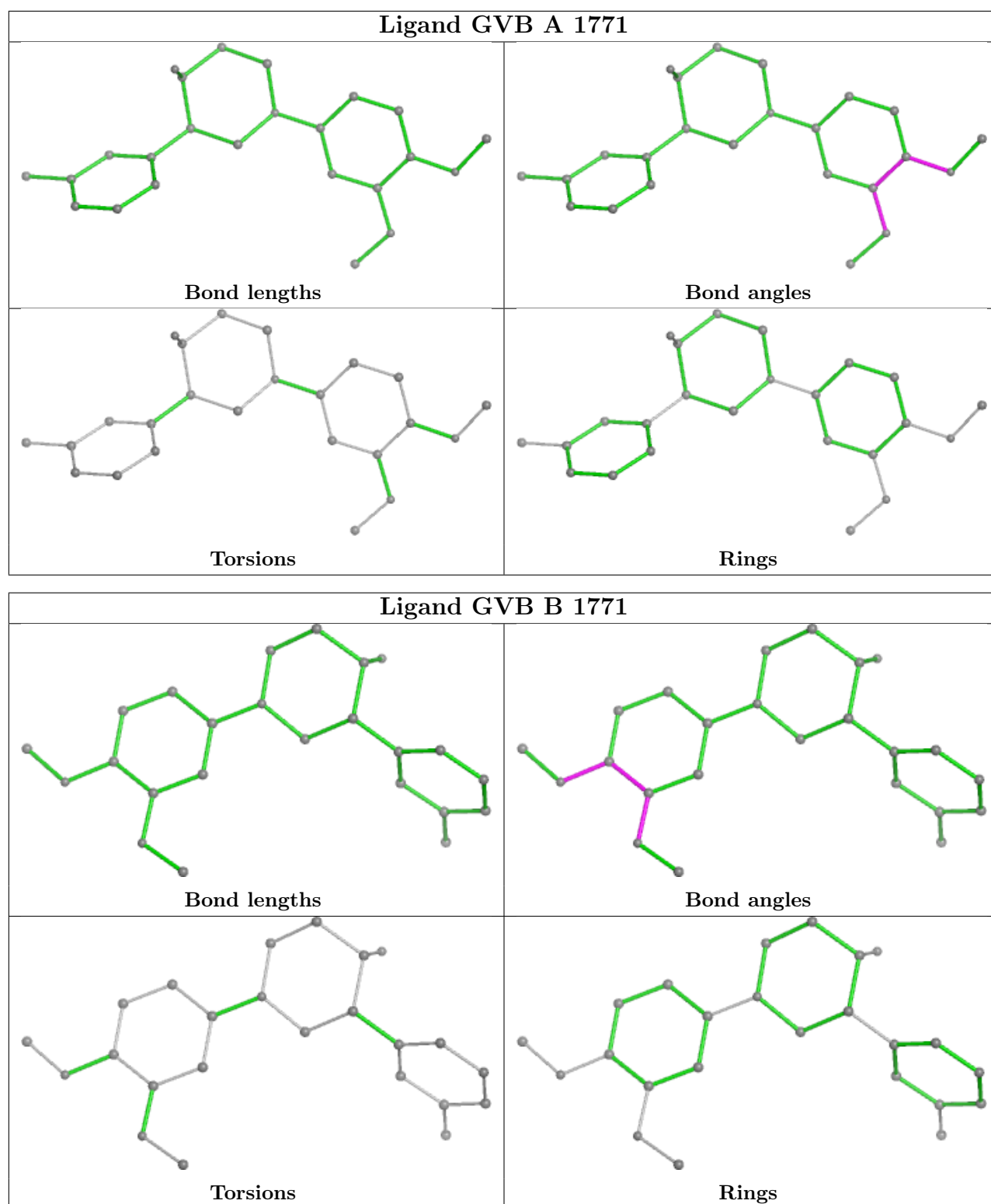
Mol	Chain	Res	Type	Atoms
2	B	1767	NAG	O7-C7-N2-C2
2	B	1770	NAG	C8-C7-N2-C2
2	B	1770	NAG	O7-C7-N2-C2
2	B	1770	NAG	O5-C5-C6-O6
2	A	1769	NAG	C8-C7-N2-C2
2	A	1769	NAG	O7-C7-N2-C2
2	A	1770	NAG	O5-C5-C6-O6
2	A	1768	NAG	O5-C5-C6-O6
2	B	1768	NAG	C8-C7-N2-C2
2	B	1767	NAG	C1-C2-N2-C7
2	B	1768	NAG	O7-C7-N2-C2
2	B	1770	NAG	C4-C5-C6-O6
2	A	1770	NAG	C4-C5-C6-O6
2	A	1768	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 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1767	NAG	4	0
2	B	1769	NAG	3	0
2	A	1769	NAG	2	0
3	A	1771	GVB	3	0
3	B	1771	GVB	5	0
2	A	1768	NAG	4	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 ⓘ

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.