



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:00 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.; Luebbers, 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

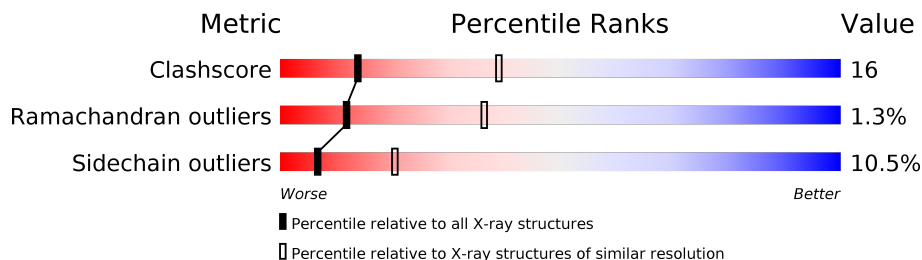
1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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](#)

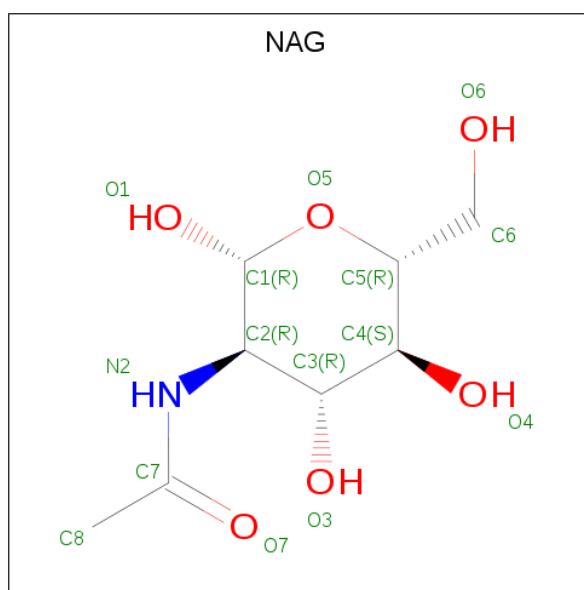
There are 4 unique types of molecules in this entry. The entry contains 12214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0
1	B	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0

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



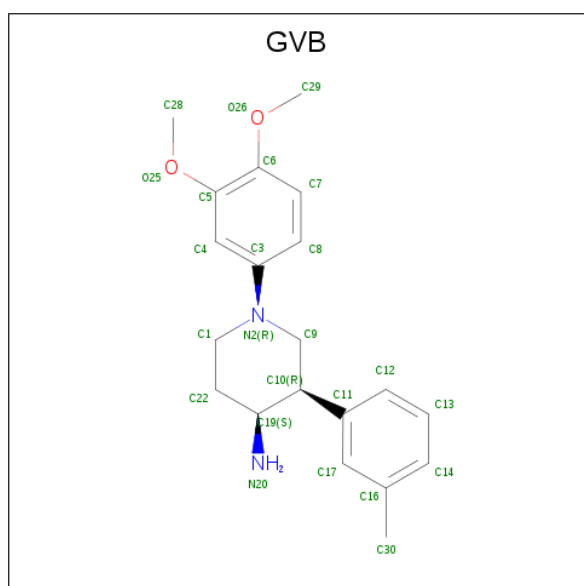
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0

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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.

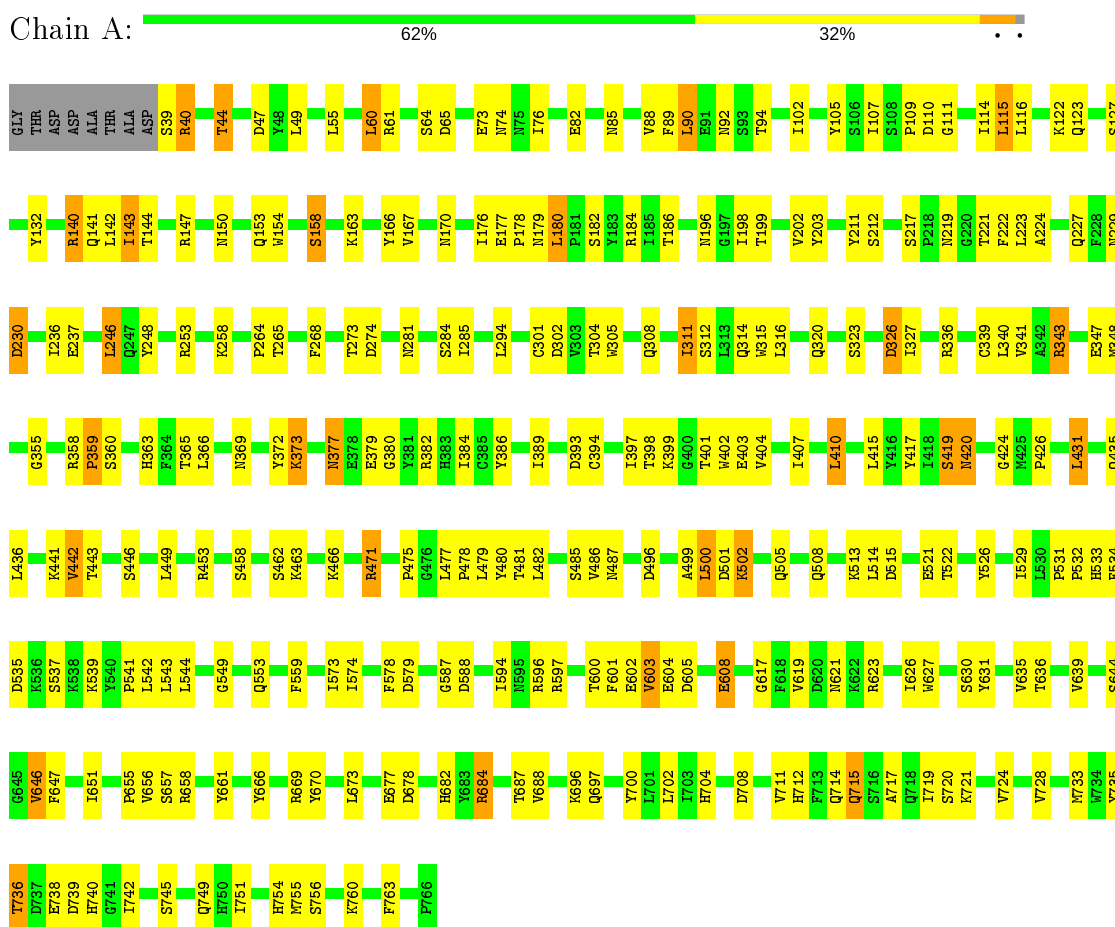
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	73	Total	O	0	0
			73	73		

3 Residue-property plots [i](#)

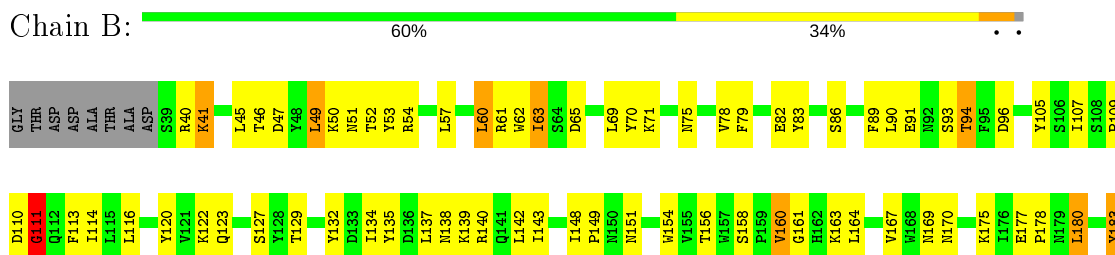
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: DIPEPTIDYL PEPTIDASE 4



V698	V699	Y700	N710	H711	H712	F713	Q714	Q715	S716	A717	D725	V726	G727	V728	D729	Y735	T736	G741	I742	Q749	H750	I751	Y752	T753	H754	N755	K760	Q761	C762	F763	S764	L765	P766	C699	T600	F601	E602	V603	Q606	R611	S614	K615	F618	V619	D620	M621	K622	R623	I624	A625	I626	W627	S630	V635	T636	S637	M638	V639	K648	C649	G650	S657	R658	D663	Y666	R669	T675	D678	M679	L680	D681	H682	Y683	R684	T687	F695	K696	Q697	R492	L500	N506	M509	P510	K513	L514	T515	F516	I517	I518	L519	M520	K523	Q527	D535	K538	P541	L542	L543	L544	P550	C551	V558	M562	W563	A564	T565	Y566	L567	E571	F578	D579	G582	Y585	M591	H592	A593	I594	R597	L598	E378	E379	G380	Y381	C385	Y386	F387	Q388	I389	K392	K399	G400	T401	W402	E403	W404	I405	S412	D413	Y414	L415	Y416	Y417	Q414	M420	E421	R429	K433	I434	Q435	K441	M450	R453	C454	Y457	S462	K463	E464	L470	R471	C472	P478	L479	Y480	T481	L482	H483	Y979	T280	T283	S284	T288	A289	P290	M293	L294	I295	H298	Y299	L300	C301	D302	W305	A306	R310	I311	S312	L313	Q314	W315	L316	R317	R318	I319	Q320	E244	V324	M325	D326	I327	C328	D329	L340	V341	A342	R343	T350	T351	P359	P362	T365	Y372	K373	N377	I193	I194	Y195	I198	W201	V202	F208	S209	L214	N219	G220	T221	F222	L223	A224	Y225	A226	Q227	F228	N229	P234	L235	I236	E237	S242	D243	E244	S245	L246	Q247	Y248	P249	V252	R253	K258	N263	V266	K267	F268	F269	V271	N272	T273	L276	S277	S278	Y279	T280	T283	S284	T288	A289	P290	M293	L294	I295	H298	Y299	L300	C301	D302	W305	A306	R310	I311	S312	L313	Q314	W315	L316	R317	R318	I319	Q320	E244	V324	M325	D326	I327	C328	D329	L340	V341	A342	R343	T350	T351	P359	P362	T365	Y372	K373	N377	E378	E379	G380	Y381	C385	Y386	F387	Q388	I389	K392	K399	G400	T401	W402	E403	W404	I405	S412	D413	Y414	L415	Y416	Y417	Q414	M420	E421	R429	K433	I434	Q435	K441	M450	R453	C454	Y457	S462	K463	E464	L470	R471	C472	P478	L479	Y480	T481	L482	H483	R492	L500	N506	M509	P510	K513	L514	T515	F516	I517	I518	L519	M520	K523	Q527	D535	K538	P541	L542	L543	L544	P550	C551	V558	M562	W563	A564	T565	Y566	L567	E571	F578	D579	G582	Y585	M591	H592	A593	I594	R597	L598
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4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	12214	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 [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	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:OE1	1:A:608:GLU:HA	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:HH11	1:A:140:ARG:HG3	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:N	1:A:40:ARG:HH11	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:NH1	1:A:40:ARG:H	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:147:ARG:HD2	2:A:1767:NAG:H81	1.74	0.68
1:A:39:SER:N	1:A:508:GLN:HG2	2.09	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:340:LEU:HD22	1:A:343:ARG:HH11	1.68	0.59
1:A:320:GLN:OE1	1:A:669:ARG:HG3	2.02	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:HD22	1:B:377:ASN:C	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:ND2	1:A:377:ASN:C	2.59	0.55
1:B:598:LEU:O	1:B:682:HIS:HE1	1.89	0.55
1:B:666:TYR:CZ	3:B:1771:GVB:H12	2.41	0.55
1:B:227:GLN:O	1:B:266:VAL:HA	2.07	0.55
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.07	0.55
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.42	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:O	1:B:401:THR:CG2	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:666:TYR:CE2	3:B:1771:GVB:H12	2.45	0.52
1:B:482:LEU:HD23	1:B:492:ARG:NH1	2.24	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:HD22	1:B:562:ASN:C	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:603:VAL:HG13	1:B:639:VAL:HG23	1.94	0.48
1:B:541:PRO:HG3	1:B:623:ARG:CZ	2.43	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:594:ILE:HD11	1:B:602:GLU:H	1.78	0.48
1:B:538:LYS:O	1:B:618:PHE:HA	2.13	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:446:SER:HA	1:A:449:LEU:CD1	2.44	0.48
1:A:65:ASP:HB2	1:A:466:LYS:HG3	1.96	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:N	1:A:602:GLU:OE1	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:657:SER:H	1:A:715:GLN:NE2	2.13	0.47
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.49	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:C	1:A:526:TYR:CD2	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:C	1:A:415:LEU:HD23	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:OD1	1:A:739:ASP:C	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:CG1	1:A:88:VAL:O	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:HA	1:A:431:LEU:HD23	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: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:A:76:ILE:HD12	1:A:90:LEU:HD12	1.99	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:543:LEU:HD12	1:B:567:LEU:CD1	2.48	0.43
1:B:82:GLU:HG3	1:B:83:TYR:CD2	2.53	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:CD1	1:B:183:TYR:N	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:564:ALA:O	1:B:565:THR:C	2.56	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: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:HG22	1:A:529:ILE:O	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:397:ILE:HG13	1:A:398:THR:HG23	2.01	0.42
1:A:74:ASN:HB2	1:A:92:ASN:CB	2.49	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:A:65:ASP:HA	1:A:463:LYS:O	2.19	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:B:169:ASN:O	1:B:170:ASN:HB2	2.20	0.41
1:A:754:HIS:ND1	1:B:729:ASP:OD1	2.34	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: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:65:ASP:N	1:B:65:ASP:OD1	2.49	0.41
1:A:384:ILE:HG13	1:A:404:VAL:HG21	2.03	0.41
1:A:436:LEU:HA	1:A:436:LEU:HD23	1.84	0.41
1:A:403:GLU:OE2	1:A:587:GLY:HA2	2.20	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:HG3	1:A:471:ARG:O	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:310:ARG:NE	1:B:329:ASP:OD1	2.49	0.40
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.85	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%)	13	39
1	B	726/736 (99%)	637 (88%)	79 (11%)	10 (1%)	11	34
All	All	1452/1472 (99%)	1276 (88%)	157 (11%)	19 (1%)	12	36

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%)	584 (89%)	69 (11%)	6	20
1	B	653/658 (99%)	585 (90%)	68 (10%)	7	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1306/1316 (99%)	1169 (90%)	137 (10%)	7 20

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

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

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	1768	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1767	-	-	5/6/23/26	0/1/1/1
2	NAG	A	1769	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1770	1	-	4/6/23/26	0/1/1/1
3	GVB	B	1771	-	-	0/12/25/25	0/3/3/3
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	B	1769	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1767	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1768	1	-	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	1770	NAG	C8-C7-N2-C2

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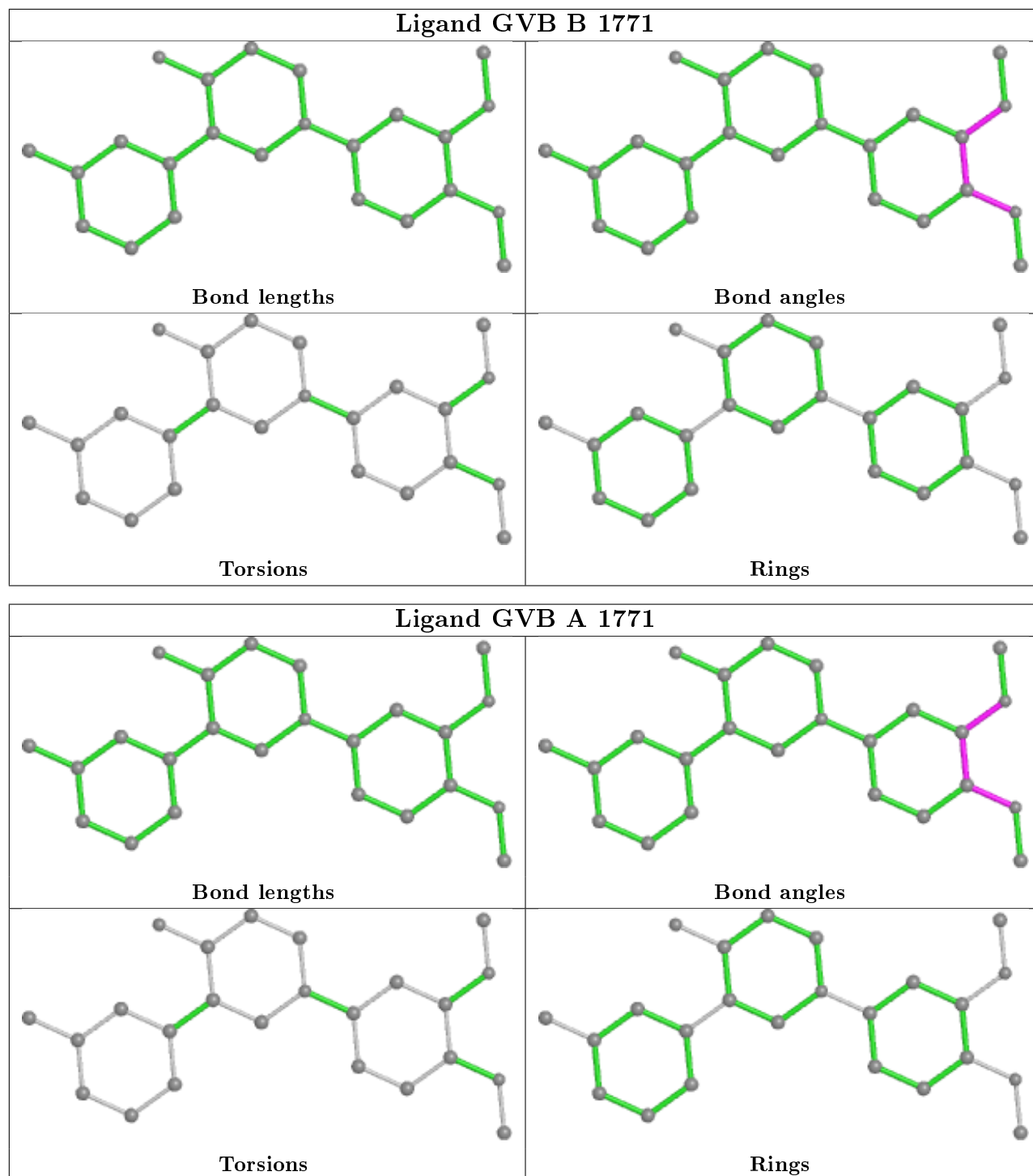
Mol	Chain	Res	Type	Atoms
2	B	1770	NAG	O7-C7-N2-C2
2	B	1767	NAG	C8-C7-N2-C2
2	B	1767	NAG	O7-C7-N2-C2
2	B	1770	NAG	O5-C5-C6-O6
2	A	1769	NAG	C8-C7-N2-C2
2	A	1769	NAG	O7-C7-N2-C2
2	A	1770	NAG	O5-C5-C6-O6
2	A	1768	NAG	O5-C5-C6-O6
2	B	1768	NAG	C8-C7-N2-C2
2	B	1767	NAG	C1-C2-N2-C7
2	B	1768	NAG	O7-C7-N2-C2
2	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	1768	NAG	4	0
2	A	1767	NAG	4	0
2	A	1769	NAG	2	0
3	B	1771	GVB	5	0
3	A	1771	GVB	3	0
2	B	1769	NAG	3	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.