



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2016 – 04:52 PM EDT

PDB ID : 1VIW
Title : TENEBRIO MOLITOR ALPHA-AMYLASE-INHIBITOR COMPLEX
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Deposited on : 1998-07-21
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

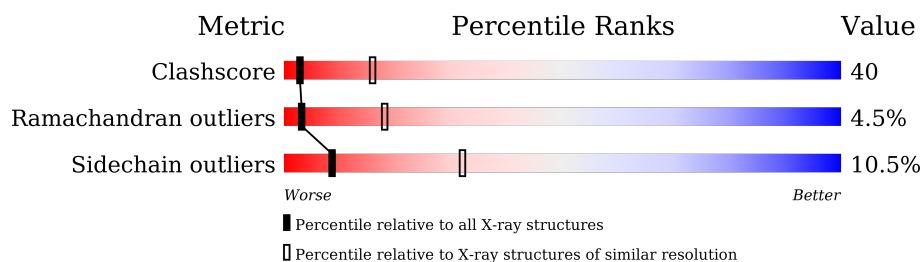
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	
2	B	205	

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
1	PCA	A	1	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5218 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 ALPHA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3604	2240	627	717	20			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ASN	ASP	CONFLICT	UNP P56634
A	158	ALA	GLN	CONFLICT	UNP P56634
A	200	ASP	SER	CONFLICT	UNP P56634

- Molecule 2 is a protein called ALPHA-AMYLASE-INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	198	Total	C	N	O	S	0	0	0
			1556	976	255	323	2			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

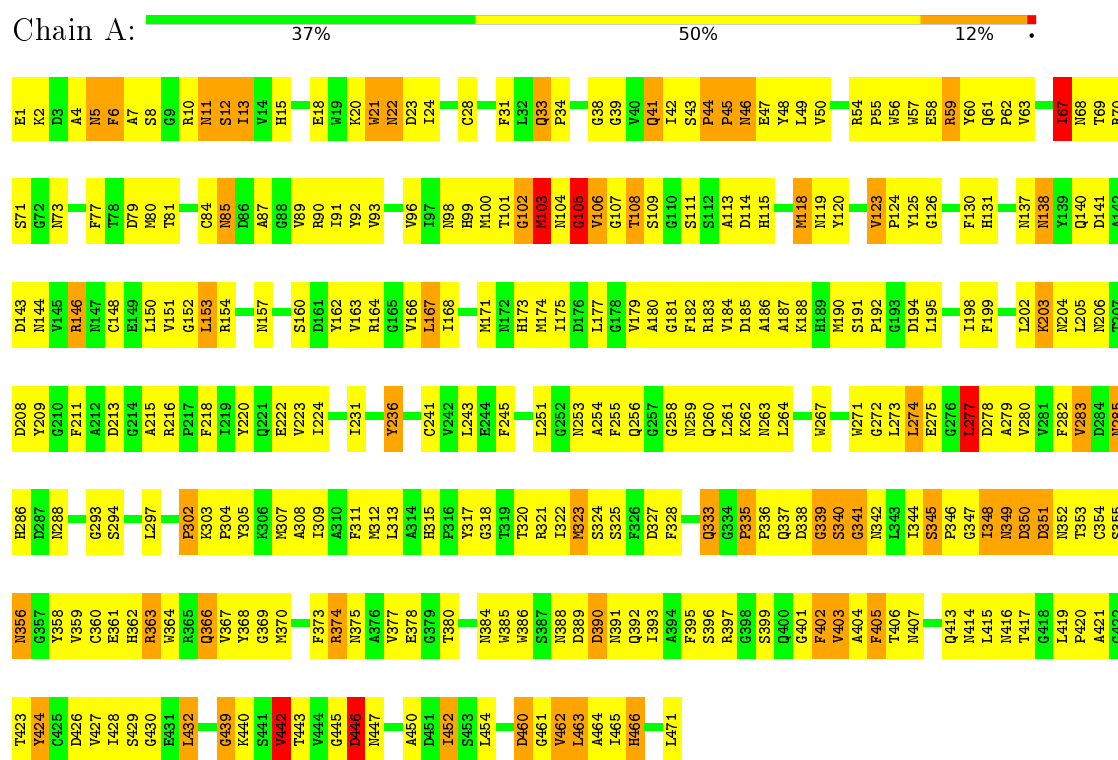
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

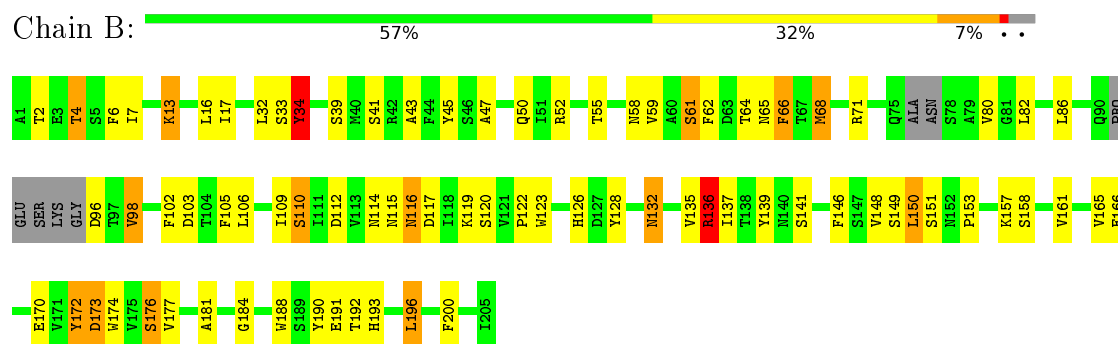
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: ALPHA-AMYLASE



• Molecule 2: ALPHA-AMYLASE-INHIBITOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.47Å 75.91Å 61.99Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.2 (10.00-3.00)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.230 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5218	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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: CA, PCA, NAG, CL

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	0.85	11/3682 (0.3%)	1.08	29/5001 (0.6%)
2	B	0.72	1/1588 (0.1%)	0.95	4/2162 (0.2%)
All	All	0.81	12/5270 (0.2%)	1.04	33/7163 (0.5%)

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	A	1	2
2	B	0	2
All	All	1	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	VAL	N-CA	-10.76	1.24	1.46
1	A	442	VAL	C-O	-8.82	1.06	1.23
1	A	349	ASN	C-N	-8.32	1.15	1.34
1	A	182	PHE	CA-C	-6.94	1.34	1.52
1	A	424	TYR	C-N	6.89	1.49	1.34
1	A	349	ASN	N-CA	-6.67	1.33	1.46
1	A	123	VAL	CA-CB	6.39	1.68	1.54
1	A	439	GLY	N-CA	5.54	1.54	1.46
2	B	116	ASN	C-O	5.24	1.33	1.23
1	A	106	VAL	N-CA	5.22	1.56	1.46
1	A	424	TYR	N-CA	-5.16	1.36	1.46
1	A	203	LYS	CE-NZ	5.10	1.61	1.49

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLY	N-CA-C	-9.77	88.67	113.10
1	A	183	ARG	N-CA-C	-9.04	86.60	111.00
1	A	341	GLY	CA-C-N	-8.30	98.93	117.20
1	A	294	SER	N-CA-C	8.30	133.41	111.00
2	B	136	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	443	THR	N-CA-CB	-7.40	96.24	110.30
1	A	104	ASN	O-C-N	7.33	135.66	123.20
1	A	146	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	104	ASN	C-N-CA	6.99	136.98	122.30
1	A	104	ASN	CA-C-N	-6.95	102.29	116.20
1	A	363	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	349	ASN	O-C-N	-6.70	111.98	122.70
2	B	176	SER	O-C-N	-6.66	112.04	122.70
1	A	105	GLY	N-CA-C	6.55	129.47	113.10
1	A	337	GLN	C-N-CA	6.12	137.01	121.70
1	A	442	VAL	CB-CA-C	-5.93	100.14	111.40
1	A	351	ASP	N-CA-C	-5.78	95.39	111.00
2	B	61	SER	O-C-N	-5.78	113.45	122.70
1	A	123	VAL	N-CA-C	5.71	126.41	111.00
1	A	118	MET	CG-SD-CE	5.67	109.27	100.20
1	A	183	ARG	N-CA-CB	5.49	120.48	110.60
1	A	374	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	B	176	SER	CA-C-O	-5.45	108.66	120.10
1	A	11	ASN	O-C-N	5.43	131.38	122.70
1	A	41	GLN	N-CA-C	-5.39	96.45	111.00
1	A	103	MET	CG-SD-CE	5.29	108.67	100.20
1	A	345	SER	C-N-CD	5.24	139.41	128.40
1	A	277	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	102	GLY	C-N-CA	5.07	134.38	121.70
1	A	378	GLU	CA-C-N	-5.07	106.07	116.20
1	A	363	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	341	GLY	O-C-N	5.04	130.76	122.70
1	A	442	VAL	CA-C-O	-5.00	109.60	120.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	PCA	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	442	VAL	Mainchain
2	B	116	ASN	Mainchain
2	B	176	SER	Mainchain

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	3604	0	3329	337	0
2	B	1556	0	1463	65	0
3	B	56	0	50	3	0
4	A	1	0	0	1	0
5	A	1	0	0	0	0
All	All	5218	0	4842	398	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 40.

All (398) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG11	1:A:125:TYR:CE2	1.59	1.38
1:A:123:VAL:HG21	1:A:125:TYR:CD2	1.74	1.22
1:A:123:VAL:HG11	1:A:125:TYR:CD2	1.76	1.19
1:A:123:VAL:HG21	1:A:125:TYR:CE2	1.87	1.09
1:A:61:GLN:HB3	1:A:101:THR:HG22	1.31	1.09
1:A:432:LEU:HD12	1:A:432:LEU:O	1.50	1.08
1:A:348:ILE:HD12	1:A:349:ASN:N	1.74	1.03
1:A:345:SER:HB3	1:A:358:TYR:CD2	1.95	1.00
1:A:123:VAL:CG1	1:A:125:TYR:CE2	2.46	0.99
1:A:123:VAL:CG2	1:A:125:TYR:CD2	2.45	0.98
1:A:123:VAL:CG1	1:A:125:TYR:CD2	2.47	0.97
1:A:274:LEU:HD21	1:A:279:ALA:HB2	1.46	0.97
1:A:349:ASN:O	1:A:350:ASP:HB2	1.66	0.94
1:A:421:ALA:HB2	1:A:446:ASP:HA	1.47	0.94
1:A:123:VAL:CG2	1:A:125:TYR:HD2	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:HH21	1:A:342:ASN:HD21	1.15	0.93
1:A:313:LEU:HD23	1:A:370:MET:HB3	1.50	0.90
1:A:364:TRP:HB3	1:A:366:GLN:HE22	1.37	0.89
1:A:102:GLY:HA2	1:A:115:HIS:CD2	2.08	0.88
1:A:442:VAL:O	1:A:442:VAL:HG23	1.72	0.88
1:A:338:ASP:OD1	1:A:338:ASP:O	1.90	0.88
2:B:86:LEU:HB2	2:B:98:VAL:HG13	1.56	0.88
1:A:123:VAL:CB	1:A:125:TYR:CD2	2.57	0.86
1:A:47:GLU:HG3	1:A:108:THR:HG22	1.57	0.86
1:A:349:ASN:O	1:A:350:ASP:CB	2.18	0.86
1:A:123:VAL:CB	1:A:125:TYR:HD2	1.89	0.85
1:A:432:LEU:O	1:A:432:LEU:CD1	2.23	0.85
1:A:346:PRO:HD2	1:A:356:ASN:HD21	1.43	0.83
1:A:427:VAL:HA	1:A:430:GLY:O	1.77	0.82
1:A:426:ASP:O	1:A:430:GLY:O	1.96	0.82
1:A:420:PRO:O	1:A:424:TYR:OH	1.98	0.81
2:B:110:SER:HB3	2:B:120:SER:HB3	1.61	0.80
1:A:364:TRP:HB3	1:A:366:GLN:NE2	1.95	0.79
1:A:262:LYS:HA	1:A:393:ILE:HD11	1.65	0.79
1:A:452:ILE:H	1:A:452:ILE:HD13	1.45	0.79
1:A:364:TRP:HB2	1:A:367:VAL:HG12	1.65	0.79
1:A:114:ASP:HB3	1:A:119:ASN:HB2	1.65	0.78
1:A:347:GLY:HA2	1:A:354:CYS:HA	1.66	0.77
1:A:93:VAL:HG23	1:A:179:VAL:HG11	1.64	0.77
2:B:136:ARG:NH2	3:B:509:NAG:H3	1.99	0.76
1:A:335:PRO:HB2	1:A:336:PRO:HD2	1.67	0.76
1:A:424:TYR:O	1:A:442:VAL:HG22	1.84	0.76
1:A:120:TYR:HB2	1:A:125:TYR:HB2	1.68	0.76
2:B:109:ILE:HG13	2:B:123:TRP:CD1	2.21	0.75
1:A:421:ALA:CB	1:A:446:ASP:HA	2.16	0.75
1:A:12:SER:O	1:A:38:GLY:N	2.19	0.74
1:A:442:VAL:CG2	1:A:442:VAL:O	2.32	0.74
1:A:348:ILE:CD1	1:A:349:ASN:N	2.50	0.73
1:A:10:ARG:HA	1:A:375:ASN:ND2	2.04	0.73
1:A:348:ILE:O	1:A:349:ASN:C	2.26	0.72
2:B:68:MET:SD	2:B:82:LEU:HD23	2.29	0.72
1:A:70:ARG:NH2	1:A:342:ASN:HD21	1.85	0.72
1:A:63:VAL:HG21	1:A:107:GLY:HA2	1.71	0.72
1:A:123:VAL:CG2	1:A:125:TYR:CE2	2.67	0.72
1:A:402:PHE:HD1	1:A:465:ILE:HG12	1.55	0.72
1:A:366:GLN:HE21	1:A:366:GLN:N	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:HD12	1:A:349:ASN:H	1.55	0.71
2:B:86:LEU:HD23	2:B:177:VAL:HG12	1.71	0.71
1:A:151:VAL:HG12	1:A:151:VAL:O	1.89	0.71
1:A:377:VAL:O	1:A:380:THR:HG23	1.89	0.71
1:A:413:GLN:HB3	1:A:452:ILE:HD11	1.73	0.70
1:A:124:PRO:HD2	1:A:162:TYR:OH	1.92	0.70
1:A:440:LYS:HE3	1:A:442:VAL:HG12	1.71	0.70
1:A:380:THR:OG1	1:A:397:ARG:HB3	1.91	0.70
1:A:33:GLN:HE21	1:A:87:ALA:HB1	1.56	0.70
1:A:338:ASP:O	1:A:340:SER:N	2.24	0.70
1:A:335:PRO:CB	1:A:336:PRO:HD2	2.21	0.69
1:A:11:ASN:HB2	1:A:375:ASN:OD1	1.93	0.69
1:A:370:MET:O	1:A:373:PHE:HB3	1.93	0.68
1:A:274:LEU:HD22	1:A:274:LEU:N	2.06	0.68
2:B:110:SER:HB3	2:B:120:SER:CB	2.24	0.68
1:A:137:ASN:HB2	1:A:144:ASN:ND2	2.09	0.68
1:A:192:PRO:HA	1:A:195:LEU:HB2	1.75	0.67
2:B:146:PHE:HB2	2:B:165:VAL:HG12	1.75	0.67
1:A:31:PHE:CD2	1:A:363:ARG:HD3	2.30	0.67
1:A:63:VAL:HG11	1:A:107:GLY:HA3	1.77	0.67
1:A:70:ARG:HH21	1:A:342:ASN:ND2	1.89	0.67
1:A:137:ASN:HB2	1:A:144:ASN:HD21	1.58	0.66
1:A:4:ALA:O	1:A:5:ASN:HB2	1.95	0.66
1:A:348:ILE:CG1	1:A:349:ASN:H	2.08	0.66
1:A:348:ILE:CD1	1:A:349:ASN:H	2.09	0.66
1:A:262:LYS:HD2	1:A:389:ASP:HA	1.78	0.66
1:A:423:THR:HG23	1:A:442:VAL:O	1.96	0.66
1:A:160:SER:O	1:A:164:ARG:HG3	1.95	0.66
1:A:49:LEU:HD12	1:A:106:VAL:O	1.95	0.66
1:A:271:TRP:HB2	1:A:273:LEU:HD13	1.77	0.65
1:A:340:SER:OG	1:A:340:SER:O	2.09	0.65
1:A:362:HIS:CD2	1:A:363:ARG:HG2	2.32	0.65
1:A:96:VAL:HA	1:A:185:ASP:HB3	1.79	0.65
1:A:81:THR:O	1:A:85:ASN:HB2	1.97	0.65
1:A:336:PRO:HG2	1:A:358:TYR:CZ	2.33	0.64
2:B:136:ARG:HH21	3:B:509:NAG:H3	1.60	0.64
1:A:204:ASN:HD22	1:A:216:ARG:HH11	1.45	0.64
1:A:366:GLN:NE2	1:A:366:GLN:H	1.96	0.64
1:A:267:TRP:CD1	1:A:311:PHE:HE2	2.16	0.64
1:A:328:PHE:HB2	1:A:333:GLN:HE22	1.63	0.64
1:A:31:PHE:O	1:A:34:PRO:HD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLN:HG2	1:A:406:THR:HB	1.80	0.64
2:B:151:SER:HA	2:B:157:LYS:O	1.98	0.64
1:A:274:LEU:HD22	1:A:274:LEU:H	1.63	0.64
1:A:105:GLY:HA2	1:A:113:ALA:O	1.97	0.63
1:A:347:GLY:O	1:A:348:ILE:HD13	1.98	0.63
1:A:396:SER:HB2	1:A:401:GLY:O	1.99	0.63
1:A:138:ASN:OD1	1:A:140:GLN:HB2	1.98	0.63
1:A:348:ILE:HG23	1:A:349:ASN:N	2.14	0.63
2:B:52:ARG:CZ	2:B:170:GLU:HA	2.29	0.63
1:A:361:GLU:O	1:A:367:VAL:HG11	1.98	0.63
1:A:283:VAL:HG21	1:A:309:ILE:HG22	1.80	0.62
1:A:164:ARG:O	1:A:168:ILE:HG13	1.98	0.62
2:B:146:PHE:HD2	2:B:165:VAL:HG11	1.65	0.62
1:A:324:SER:OG	1:A:360:CYS:HA	1.98	0.62
1:A:452:ILE:N	1:A:452:ILE:HD13	2.15	0.62
1:A:253:ASN:OD1	1:A:258:GLY:HA3	2.00	0.62
1:A:48:TYR:OH	1:A:70:ARG:HG3	2.00	0.62
1:A:102:GLY:HA2	1:A:115:HIS:HD2	1.63	0.61
1:A:93:VAL:CG2	1:A:179:VAL:HG11	2.29	0.61
1:A:364:TRP:HB2	1:A:367:VAL:CG1	2.31	0.61
1:A:427:VAL:CA	1:A:430:GLY:O	2.47	0.61
1:A:304:PRO:HA	1:A:307:MET:SD	2.42	0.60
1:A:55:PRO:O	1:A:58:GLU:HG2	2.01	0.60
2:B:146:PHE:CD2	2:B:165:VAL:HG11	2.35	0.60
1:A:61:GLN:CB	1:A:101:THR:HG22	2.19	0.60
1:A:163:VAL:O	1:A:167:LEU:HD22	2.01	0.60
1:A:335:PRO:CB	1:A:336:PRO:CD	2.80	0.60
1:A:220:TYR:CD2	1:A:243:LEU:HD21	2.36	0.60
1:A:386:TRP:CD2	1:A:415:LEU:HD21	2.37	0.60
2:B:196:LEU:N	2:B:196:LEU:HD23	2.16	0.60
1:A:397:ARG:HH11	1:A:397:ARG:HG3	1.67	0.60
1:A:322:ILE:N	1:A:322:ILE:HD12	2.17	0.60
2:B:150:LEU:O	2:B:158:SER:HA	2.01	0.60
1:A:93:VAL:HG21	1:A:174:MET:CE	2.33	0.59
1:A:31:PHE:CE1	1:A:352:ASN:ND2	2.70	0.59
1:A:402:PHE:CD1	1:A:465:ILE:HG12	2.37	0.59
1:A:93:VAL:HG21	1:A:174:MET:HE2	1.85	0.59
2:B:62:PHE:CZ	2:B:86:LEU:HD11	2.37	0.59
1:A:13:ILE:HG12	1:A:321:ARG:HG3	1.83	0.59
1:A:405:PHE:HB3	1:A:461:GLY:O	2.01	0.59
1:A:42:ILE:HD12	1:A:80:MET:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLY:C	1:A:273:LEU:HD12	2.23	0.58
1:A:313:LEU:HD23	1:A:370:MET:CB	2.28	0.58
1:A:49:LEU:HD12	1:A:50:VAL:H	1.68	0.58
1:A:461:GLY:O	1:A:462:VAL:HB	2.04	0.58
2:B:146:PHE:HB2	2:B:165:VAL:CG1	2.34	0.58
2:B:181:ALA:HB1	2:B:193:HIS:ND1	2.19	0.57
1:A:262:LYS:HD2	1:A:389:ASP:CA	2.34	0.57
1:A:39:GLY:HA2	1:A:89:VAL:HG13	1.86	0.57
1:A:328:PHE:CB	1:A:333:GLN:HE22	2.17	0.57
1:A:131:HIS:CE1	1:A:157:ASN:HA	2.40	0.57
1:A:205:LEU:HD13	1:A:211:PHE:CD1	2.39	0.56
1:A:243:LEU:HD23	1:A:280:VAL:HB	1.87	0.56
1:A:399:SER:O	1:A:419:LEU:HG	2.05	0.56
2:B:86:LEU:CD2	2:B:177:VAL:HG12	2.34	0.56
1:A:124:PRO:HD2	1:A:162:TYR:HH	1.71	0.56
1:A:427:VAL:HG22	1:A:464:ALA:HB3	1.87	0.56
2:B:96:ASP:N	2:B:114:ASN:ND2	2.53	0.56
1:A:465:ILE:O	1:A:465:ILE:HG13	2.06	0.56
1:A:130:PHE:CE2	1:A:154:ARG:HB3	2.41	0.55
1:A:302:PRO:O	1:A:305:TYR:HB3	2.06	0.55
1:A:348:ILE:CG1	1:A:349:ASN:N	2.69	0.55
1:A:123:VAL:HB	1:A:125:TYR:HD2	1.69	0.55
1:A:181:GLY:HA2	1:A:218:PHE:O	2.06	0.55
1:A:391:ASN:HB3	1:A:407:ASN:HB2	1.88	0.55
1:A:274:LEU:CD2	1:A:279:ALA:HB2	2.30	0.55
1:A:359:VAL:HB	1:A:361:GLU:OE1	2.07	0.55
1:A:391:ASN:O	1:A:406:THR:HA	2.07	0.54
1:A:7:ALA:HB3	1:A:10:ARG:HD2	1.88	0.54
1:A:166:VAL:HG23	1:A:167:LEU:N	2.23	0.54
1:A:272:GLY:O	1:A:273:LEU:HD12	2.07	0.54
2:B:148:VAL:HB	2:B:161:VAL:HG12	1.90	0.54
1:A:164:ARG:NH2	1:A:194:ASP:HB3	2.23	0.54
1:A:243:LEU:HB3	1:A:282:PHE:CE1	2.43	0.54
1:A:344:ILE:HG22	1:A:345:SER:N	2.23	0.54
1:A:123:VAL:HG21	1:A:125:TYR:HE2	1.63	0.54
2:B:109:ILE:HD11	2:B:150:LEU:HD12	1.90	0.54
2:B:126:HIS:CD2	2:B:126:HIS:O	2.60	0.54
1:A:385:TRP:CZ2	1:A:393:ILE:HD12	2.43	0.53
1:A:103:MET:H	1:A:115:HIS:CD2	2.27	0.53
1:A:77:PHE:CZ	1:A:174:MET:HE1	2.43	0.53
2:B:151:SER:O	2:B:153:PRO:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:HZ2	1:A:45:PRO:HA	1.72	0.53
1:A:346:PRO:HG2	1:A:355:SER:OG	2.08	0.53
2:B:50:GLN:HB2	2:B:174:TRP:CZ3	2.44	0.53
2:B:17:ILE:O	2:B:43:ALA:HA	2.08	0.53
1:A:102:GLY:HA2	1:A:115:HIS:NE2	2.24	0.53
1:A:251:LEU:O	1:A:255:PHE:HD1	1.91	0.53
1:A:328:PHE:HB2	1:A:333:GLN:NE2	2.24	0.53
1:A:348:ILE:HD12	1:A:348:ILE:C	2.25	0.53
2:B:135:VAL:HA	2:B:149:SER:O	2.08	0.53
1:A:415:LEU:HD12	1:A:452:ILE:CD1	2.39	0.53
1:A:220:TYR:CE2	1:A:243:LEU:HD21	2.44	0.53
2:B:128:TYR:CE1	2:B:150:LEU:HD22	2.44	0.52
1:A:24:ILE:HG22	1:A:28:CYS:SG	2.50	0.52
1:A:336:PRO:CG	1:A:358:TYR:CZ	2.93	0.52
1:A:62:PRO:HD2	1:A:100:MET:O	2.09	0.52
1:A:243:LEU:HB3	1:A:282:PHE:HE1	1.75	0.52
1:A:426:ASP:O	1:A:430:GLY:C	2.47	0.52
1:A:12:SER:CB	1:A:320:THR:OG1	2.58	0.51
1:A:84:CYS:SG	1:A:91:ILE:HD11	2.51	0.51
1:A:15:HIS:HD2	1:A:323:MET:SD	2.34	0.51
1:A:254:ALA:HA	1:A:259:ASN:HB3	1.91	0.51
1:A:428:ILE:HG13	1:A:462:VAL:HG13	1.93	0.51
1:A:31:PHE:C	1:A:34:PRO:HD2	2.31	0.51
2:B:114:ASN:O	2:B:115:ASN:HB2	2.10	0.50
1:A:336:PRO:HG2	1:A:358:TYR:OH	2.11	0.50
1:A:429:SER:OG	1:A:430:GLY:N	2.45	0.50
2:B:136:ARG:HH21	3:B:509:NAG:C3	2.25	0.50
1:A:60:TYR:O	1:A:99:HIS:HE1	1.94	0.50
1:A:107:GLY:HA3	1:A:111:SER:O	2.12	0.50
1:A:2:LYS:HB3	1:A:241:CYS:SG	2.52	0.50
2:B:13:LYS:N	2:B:13:LYS:HD2	2.27	0.50
1:A:150:LEU:O	1:A:153:LEU:HB2	2.12	0.50
1:A:198:ILE:O	1:A:202:LEU:HD13	2.12	0.50
1:A:366:GLN:NE2	1:A:366:GLN:N	2.53	0.49
2:B:196:LEU:HD23	2:B:196:LEU:H	1.76	0.49
1:A:364:TRP:CB	1:A:367:VAL:HG12	2.40	0.49
1:A:384:ASN:O	1:A:395:PHE:HA	2.12	0.49
1:A:123:VAL:HG12	1:A:124:PRO:O	2.11	0.49
1:A:338:ASP:O	1:A:339:GLY:C	2.51	0.49
1:A:67:ILE:HD11	1:A:173:HIS:HE1	1.76	0.49
2:B:128:TYR:CZ	2:B:150:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HB3	1:A:420:PRO:HD2	1.94	0.49
1:A:98:ASN:HB2	1:A:190:MET:SD	2.52	0.49
2:B:112:ASP:HA	2:B:117:ASP:HA	1.93	0.49
2:B:139:TYR:CE1	2:B:165:VAL:HG13	2.48	0.49
1:A:373:PHE:HA	1:A:466:HIS:CE1	2.48	0.49
1:A:48:TYR:CE2	1:A:59:ARG:HD2	2.47	0.49
1:A:67:ILE:HD12	1:A:67:ILE:H	1.77	0.49
1:A:335:PRO:HB2	1:A:336:PRO:CD	2.39	0.49
1:A:203:LYS:NZ	1:A:203:LYS:HB3	2.28	0.48
1:A:388:ASN:OD1	1:A:392:GLN:HB2	2.13	0.48
1:A:397:ARG:HG3	1:A:397:ARG:NH1	2.26	0.48
1:A:423:THR:CG2	1:A:424:TYR:N	2.76	0.48
1:A:77:PHE:CZ	1:A:174:MET:CE	2.96	0.48
2:B:137:ILE:HD12	2:B:148:VAL:HG22	1.94	0.48
1:A:151:VAL:CG1	1:A:151:VAL:O	2.60	0.48
1:A:11:ASN:ND2	1:A:375:ASN:HA	2.29	0.48
1:A:273:LEU:HB3	1:A:317:TYR:OH	2.14	0.48
1:A:141:ASP:OD2	1:A:144:ASN:HB2	2.13	0.47
1:A:348:ILE:O	1:A:350:ASP:N	2.46	0.47
2:B:71:ARG:HB2	2:B:192:THR:OG1	2.13	0.47
1:A:20:LYS:HE3	1:A:342:ASN:O	2.13	0.47
1:A:419:LEU:CB	1:A:420:PRO:HD2	2.45	0.47
1:A:313:LEU:HB3	1:A:370:MET:HG3	1.94	0.47
1:A:21:TRP:CH2	1:A:42:ILE:HD11	2.50	0.47
1:A:454:LEU:HD11	1:A:460:ASP:O	2.13	0.47
1:A:58:GLU:HG3	1:A:59:ARG:N	2.28	0.47
1:A:424:TYR:CD1	1:A:424:TYR:N	2.83	0.47
1:A:137:ASN:CB	1:A:144:ASN:HD21	2.26	0.47
2:B:6:PHE:C	2:B:7:ILE:HD12	2.36	0.47
1:A:18:GLU:HG3	1:A:335:PRO:HG3	1.97	0.47
1:A:415:LEU:HB2	1:A:452:ILE:HD12	1.97	0.47
1:A:92:TYR:HD1	1:A:181:GLY:HA3	1.80	0.47
1:A:286:HIS:HA	1:A:323:MET:CE	2.45	0.47
1:A:346:PRO:HD2	1:A:356:ASN:ND2	2.22	0.47
1:A:21:TRP:CZ3	1:A:42:ILE:HD11	2.49	0.47
1:A:103:MET:O	1:A:115:HIS:HB2	2.15	0.46
1:A:166:VAL:HG23	1:A:167:LEU:H	1.79	0.46
1:A:18:GLU:CG	1:A:335:PRO:HG3	2.45	0.46
2:B:7:ILE:HD12	2:B:7:ILE:N	2.30	0.46
1:A:21:TRP:CE3	1:A:71:SER:HB3	2.50	0.46
2:B:2:THR:HG22	2:B:4:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:MET:HG2	1:A:461:GLY:O	2.15	0.46
2:B:52:ARG:HB3	2:B:173:ASP:HA	1.97	0.46
1:A:22:ASN:HD22	1:A:23:ASP:N	2.12	0.46
1:A:415:LEU:O	1:A:450:ALA:N	2.49	0.46
1:A:49:LEU:HD12	1:A:50:VAL:N	2.31	0.46
2:B:177:VAL:HG11	2:B:200:PHE:CZ	2.51	0.46
1:A:125:TYR:OH	1:A:166:VAL:HG21	2.16	0.46
1:A:42:ILE:HD12	1:A:80:MET:CE	2.45	0.46
2:B:59:VAL:HG23	2:B:141:SER:HB3	1.97	0.46
1:A:151:VAL:O	1:A:153:LEU:N	2.48	0.46
1:A:188:LYS:HG3	1:A:231:ILE:HG21	1.98	0.46
1:A:417:THR:O	1:A:419:LEU:HD13	2.16	0.46
2:B:64:THR:CG2	2:B:137:ILE:HB	2.45	0.46
1:A:236:TYR:N	1:A:236:TYR:CD1	2.84	0.46
1:A:33:GLN:HE21	1:A:87:ALA:CB	2.24	0.46
1:A:370:MET:HE1	1:A:464:ALA:HB2	1.98	0.46
1:A:130:PHE:CD2	1:A:154:ARG:HB3	2.51	0.45
1:A:277:LEU:HD13	1:A:277:LEU:H	1.81	0.45
2:B:71:ARG:O	2:B:191:GLU:HG3	2.16	0.45
1:A:328:PHE:HA	1:A:333:GLN:HE22	1.82	0.45
1:A:138:ASN:C	1:A:140:GLN:H	2.19	0.45
1:A:180:ALA:HB2	1:A:211:PHE:CZ	2.51	0.45
1:A:123:VAL:HB	1:A:125:TYR:CD2	2.44	0.45
1:A:43:SER:OG	1:A:44:PRO:HD2	2.17	0.45
1:A:92:TYR:CD1	1:A:181:GLY:HA3	2.52	0.45
1:A:404:ALA:O	1:A:462:VAL:HA	2.16	0.45
1:A:6:PHE:N	1:A:6:PHE:CD1	2.83	0.45
1:A:80:MET:O	1:A:84:CYS:HB2	2.17	0.45
2:B:32:LEU:HD12	2:B:32:LEU:N	2.32	0.45
1:A:12:SER:HB2	1:A:320:THR:OG1	2.16	0.45
1:A:1:PCA:HB3	1:A:216:ARG:HB2	1.97	0.45
1:A:177:LEU:O	1:A:209:TYR:CZ	2.70	0.45
1:A:31:PHE:CG	1:A:363:ARG:HD3	2.52	0.45
1:A:321:ARG:NH2	4:A:498:CL:CL	2.86	0.45
1:A:48:TYR:CZ	1:A:59:ARG:HD2	2.52	0.45
1:A:123:VAL:HB	1:A:124:PRO:C	2.37	0.45
2:B:109:ILE:HG13	2:B:123:TRP:CG	2.52	0.45
1:A:205:LEU:HD12	1:A:215:ALA:HB3	1.99	0.45
2:B:32:LEU:HB3	2:B:41:SER:OG	2.16	0.45
1:A:13:ILE:O	1:A:321:ARG:HA	2.18	0.44
1:A:303:LYS:HE3	1:A:460:ASP:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HG21	1:A:199:PHE:CZ	2.53	0.44
1:A:274:LEU:CD2	1:A:274:LEU:N	2.78	0.44
2:B:132:ASN:O	2:B:153:PRO:HD2	2.17	0.44
1:A:256:GLN:OE1	1:A:297:LEU:HD21	2.18	0.44
1:A:402:PHE:C	1:A:402:PHE:CD1	2.89	0.44
1:A:328:PHE:CA	1:A:333:GLN:HE22	2.29	0.44
1:A:47:GLU:CD	1:A:109:SER:HB3	2.38	0.44
1:A:61:GLN:HA	1:A:100:MET:O	2.17	0.44
1:A:174:MET:O	1:A:179:VAL:HG22	2.18	0.44
1:A:68:ASN:HA	1:A:73:ASN:HA	1.99	0.44
1:A:386:TRP:CE2	1:A:415:LEU:HD21	2.52	0.44
1:A:403:VAL:HA	1:A:463:LEU:O	2.18	0.44
1:A:415:LEU:HD12	1:A:452:ILE:HD11	2.00	0.44
1:A:47:GLU:CG	1:A:108:THR:HG22	2.40	0.43
1:A:102:GLY:CA	1:A:115:HIS:HD2	2.30	0.43
1:A:206:ASN:ND2	1:A:209:TYR:CE1	2.87	0.43
1:A:187:ALA:HA	1:A:190:MET:HE3	2.00	0.43
1:A:224:ILE:HG21	2:B:39:SER:HB3	1.99	0.43
1:A:151:VAL:HG11	2:B:188:TRP:CD1	2.53	0.43
1:A:187:ALA:HB3	1:A:223:VAL:CG2	2.48	0.43
1:A:220:TYR:CB	1:A:280:VAL:HG21	2.49	0.43
1:A:368:TYR:CD1	1:A:369:GLY:N	2.87	0.43
1:A:286:HIS:HA	1:A:323:MET:HE2	2.01	0.43
1:A:471:LEU:H	1:A:471:LEU:HD23	1.84	0.43
1:A:144:ASN:O	1:A:148:CYS:HB2	2.18	0.43
1:A:323:MET:O	1:A:361:GLU:HB2	2.19	0.43
1:A:338:ASP:CG	1:A:338:ASP:O	2.55	0.43
2:B:34:TYR:CE1	2:B:192:THR:HB	2.54	0.43
2:B:45:TYR:CE2	2:B:47:ALA:HB3	2.54	0.43
1:A:20:LYS:HE3	1:A:342:ASN:HB2	2.00	0.42
1:A:423:THR:HG22	1:A:424:TYR:N	2.33	0.42
1:A:46:ASN:ND2	1:A:46:ASN:C	2.71	0.42
1:A:206:ASN:HD22	1:A:209:TYR:HE1	1.67	0.42
1:A:206:ASN:ND2	1:A:209:TYR:HE1	2.17	0.42
1:A:315:HIS:O	1:A:374:ARG:NH1	2.50	0.42
1:A:405:PHE:N	1:A:405:PHE:CD1	2.87	0.42
1:A:224:ILE:HA	1:A:245:PHE:CD2	2.54	0.42
1:A:305:TYR:O	1:A:308:ALA:HB3	2.19	0.42
2:B:80:VAL:HG22	2:B:184:GLY:HA3	2.01	0.42
1:A:118:MET:O	1:A:126:GLY:HA2	2.20	0.42
1:A:324:SER:HB2	1:A:362:HIS:ND1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLN:HB3	1:A:333:GLN:HE21	1.39	0.42
1:A:113:ALA:HB1	1:A:120:TYR:CE1	2.54	0.42
1:A:146:ARG:HD3	1:A:191:SER:HA	2.01	0.42
1:A:271:TRP:CB	1:A:273:LEU:HD13	2.47	0.42
1:A:323:MET:HE3	1:A:325:SER:HB3	2.00	0.42
1:A:367:VAL:HG13	1:A:368:TYR:H	1.84	0.42
1:A:24:ILE:HD12	1:A:80:MET:SD	2.58	0.42
1:A:373:PHE:CD2	1:A:464:ALA:HB1	2.55	0.42
1:A:54:ARG:CZ	1:A:70:ARG:HD3	2.49	0.42
1:A:171:MET:O	1:A:174:MET:HB2	2.20	0.42
1:A:388:ASN:HD21	1:A:390:ASP:HB3	1.85	0.42
2:B:114:ASN:N	2:B:114:ASN:HD22	2.17	0.42
1:A:141:ASP:HB2	2:B:115:ASN:HD21	1.83	0.42
1:A:348:ILE:CG2	1:A:349:ASN:N	2.77	0.42
1:A:406:THR:HG22	1:A:454:LEU:HD23	2.01	0.42
2:B:82:LEU:O	2:B:102:PHE:HB2	2.20	0.42
2:B:177:VAL:O	2:B:177:VAL:HG23	2.20	0.42
1:A:220:TYR:HA	1:A:241:CYS:O	2.20	0.42
1:A:220:TYR:HD2	1:A:243:LEU:HD21	1.82	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.91	0.41
1:A:351:ASP:CG	1:A:353:THR:HG23	2.40	0.41
2:B:52:ARG:NE	2:B:170:GLU:HA	2.34	0.41
1:A:373:PHE:HA	1:A:466:HIS:ND1	2.35	0.41
1:A:90:ARG:HB3	1:A:92:TYR:CE2	2.55	0.41
1:A:31:PHE:HZ	1:A:368:TYR:CD2	2.39	0.41
1:A:84:CYS:SG	1:A:89:VAL:HB	2.61	0.41
2:B:103:ASP:OD2	2:B:106:LEU:HG	2.21	0.41
2:B:65:ASN:O	2:B:66:PHE:HB3	2.20	0.41
1:A:151:VAL:HA	2:B:105:PHE:CE2	2.55	0.41
1:A:186:ALA:H	1:A:222:GLU:HB3	1.85	0.41
2:B:128:TYR:CE2	2:B:150:LEU:HD13	2.54	0.41
1:A:175:ILE:HD11	1:A:202:LEU:HG	2.03	0.41
1:A:260:GLN:HB2	1:A:263:ASN:OD1	2.20	0.41
1:A:285:ASN:O	1:A:286:HIS:C	2.58	0.41
1:A:56:TRP:CG	1:A:57:TRP:N	2.88	0.41
1:A:166:VAL:HG23	1:A:167:LEU:HD13	2.02	0.41
1:A:311:PHE:O	1:A:315:HIS:HB2	2.21	0.41
1:A:59:ARG:NH1	1:A:70:ARG:HB2	2.35	0.41
1:A:392:GLN:HA	1:A:405:PHE:O	2.21	0.41
1:A:392:GLN:HG2	1:A:406:THR:CB	2.49	0.41
1:A:402:PHE:CG	1:A:403:VAL:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:O	1:A:125:TYR:N	2.55	0.41
1:A:202:LEU:O	1:A:216:ARG:NH1	2.54	0.41
1:A:275:GLU:O	1:A:278:ASP:HB2	2.20	0.41
1:A:33:GLN:HB2	1:A:87:ALA:O	2.21	0.40
1:A:377:VAL:HG21	1:A:397:ARG:NH1	2.37	0.40
1:A:41:GLN:HA	1:A:92:TYR:HB2	2.02	0.40
1:A:42:ILE:HG23	1:A:42:ILE:O	2.21	0.40
1:A:59:ARG:HH12	1:A:70:ARG:HB2	1.87	0.40
1:A:204:ASN:ND2	1:A:204:ASN:N	2.69	0.40
1:A:264:LEU:O	1:A:267:TRP:HB2	2.21	0.40
1:A:77:PHE:O	1:A:81:THR:HG23	2.21	0.40
1:A:452:ILE:CD1	1:A:452:ILE:N	2.83	0.40
2:B:126:HIS:CG	2:B:126:HIS:O	2.74	0.40
2:B:191:GLU:HG2	2:B:193:HIS:NE2	2.36	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	469/471 (100%)	361 (77%)	83 (18%)	25 (5%)	2	14
2	B	192/205 (94%)	166 (86%)	21 (11%)	5 (3%)	7	33
All	All	661/676 (98%)	527 (80%)	104 (16%)	30 (4%)	3	18

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	MET
1	A	105	GLY
1	A	340	SER
1	A	446	ASP

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Mol	Chain	Res	Type
2	B	172	TYR
2	B	173	ASP
1	A	8	SER
1	A	152	GLY
1	A	213	ASP
1	A	339	GLY
1	A	350	ASP
1	A	462	VAL
1	A	12	SER
1	A	67	ILE
1	A	312	MET
1	A	390	ASP
2	B	34	TYR
1	A	318	GLY
1	A	5	ASN
1	A	44	PRO
1	A	208	ASP
1	A	277	LEU
1	A	302	PRO
1	A	447	ASN
2	B	58	ASN
2	B	66	PHE
1	A	335	PRO
1	A	445	GLY
1	A	283	VAL
1	A	439	GLY

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	380/380 (100%)	340 (90%)	40 (10%)	8	32
2	B	180/185 (97%)	161 (89%)	19 (11%)	8	31
All	All	560/565 (99%)	501 (90%)	59 (10%)	8	32

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	13	ILE
1	A	21	TRP
1	A	22	ASN
1	A	33	GLN
1	A	45	PRO
1	A	46	ASN
1	A	59	ARG
1	A	67	ILE
1	A	69	THR
1	A	79	ASP
1	A	85	ASN
1	A	108	THR
1	A	138	ASN
1	A	143	ASP
1	A	153	LEU
1	A	167	LEU
1	A	236	TYR
1	A	261	LEU
1	A	274	LEU
1	A	277	LEU
1	A	285	ASN
1	A	288	ASN
1	A	323	MET
1	A	327	ASP
1	A	333	GLN
1	A	348	ILE
1	A	356	ASN
1	A	366	GLN
1	A	402	PHE
1	A	403	VAL
1	A	405	PHE
1	A	414	ASN
1	A	416	ASN
1	A	432	LEU
1	A	446	ASP
1	A	452	ILE
1	A	460	ASP
1	A	463	LEU
1	A	466	HIS
2	B	4	THR
2	B	13	LYS
2	B	16	LEU

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Mol	Chain	Res	Type
2	B	33	SER
2	B	34	TYR
2	B	55	THR
2	B	61	SER
2	B	68	MET
2	B	98	VAL
2	B	110	SER
2	B	119	LYS
2	B	122	PRO
2	B	132	ASN
2	B	136	ARG
2	B	150	LEU
2	B	166	GLU
2	B	172	TYR
2	B	190	TYR
2	B	196	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	15	HIS
1	A	22	ASN
1	A	33	GLN
1	A	46	ASN
1	A	99	HIS
1	A	115	HIS
1	A	137	ASN
1	A	144	ASN
1	A	173	HIS
1	A	204	ASN
1	A	286	HIS
1	A	288	ASN
1	A	301	ASN
1	A	331	ASN
1	A	333	GLN
1	A	337	GLN
1	A	342	ASN
1	A	366	GLN
1	A	384	ASN
1	A	392	GLN
1	A	416	ASN

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Mol	Chain	Res	Type
2	B	27	ASN
2	B	31	GLN
2	B	90	GLN
2	B	114	ASN
2	B	115	ASN
2	B	126	HIS
2	B	159	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	1.18	1 (14%)	9,10,12	7.55	7 (77%)

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
1	PCA	A	1	1	1/1/2/4	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CG-CD	2.69	1.59	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CG-CD	-5.43	94.73	104.21
1	A	1	PCA	CG-CD-N	-5.05	92.93	108.28
1	A	1	PCA	CB-CA-N	-4.47	89.75	103.34
1	A	1	PCA	OE-CD-CG	-3.22	120.48	126.85
1	A	1	PCA	CG-CB-CA	-2.40	93.88	104.23
1	A	1	PCA	OE-CD-N	7.86	146.52	124.61
1	A	1	PCA	CB-CA-C	18.79	140.69	112.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	PCA	CA

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	1	0

5.5 Carbohydrates

4 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	508	3	14,14,15	0.48	0	15,19,21	1.12	1 (6%)
3	NAG	B	509	3,2	14,14,15	0.71	0	15,19,21	1.20	1 (6%)
3	NAG	B	510	3	14,14,15	1.09	1 (7%)	15,19,21	1.06	1 (6%)
3	NAG	B	511	3,2	14,14,15	0.87	1 (7%)	15,19,21	1.45	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	508	3	-	0/6/23/26	0/1/1/1
3	NAG	B	509	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	510	3	-	0/6/23/26	0/1/1/1
3	NAG	B	511	3,2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	511	NAG	C1-C2	2.02	1.55	1.52
3	B	510	NAG	C1-C2	3.32	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	511	NAG	C1-O5-C5	-4.60	105.38	112.14
3	B	509	NAG	C1-O5-C5	-3.68	106.73	112.14
3	B	508	NAG	C1-O5-C5	-3.59	106.87	112.14
3	B	510	NAG	C1-O5-C5	-3.34	107.23	112.14
3	B	511	NAG	C2-N2-C7	-2.56	119.78	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	509	NAG	3	0

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.