



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:16 AM GMT

PDB ID : 2WIL  
Title : AGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED  
BY TABUN ANALOGUE TA5  
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Deposited on : 2009-05-12  
Resolution : 3.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

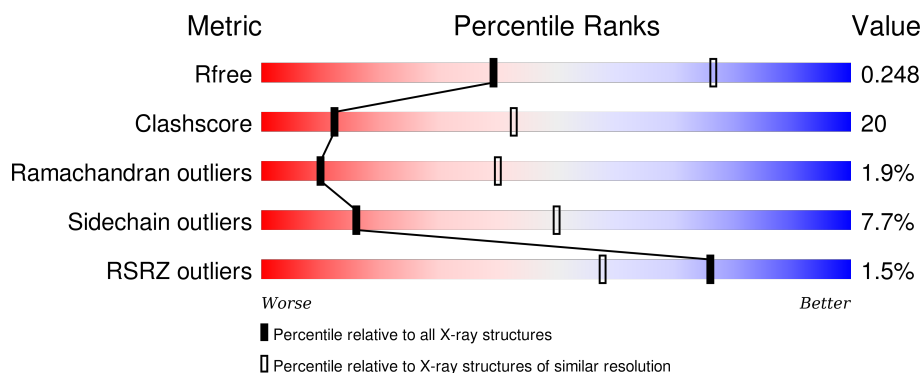
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	529	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 63%, green 32%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>63%</span> <span>32%</span> <span>• •</span> </div> </div>
1	B	529	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 59%, green 36%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>59%</span> <span>36%</span> <span>• •</span> </div> </div>

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
3	FUC	A	1533	-	-	-	X
3	FUC	B	1533	-	-	-	X
4	NAG	A	1539	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8798 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.

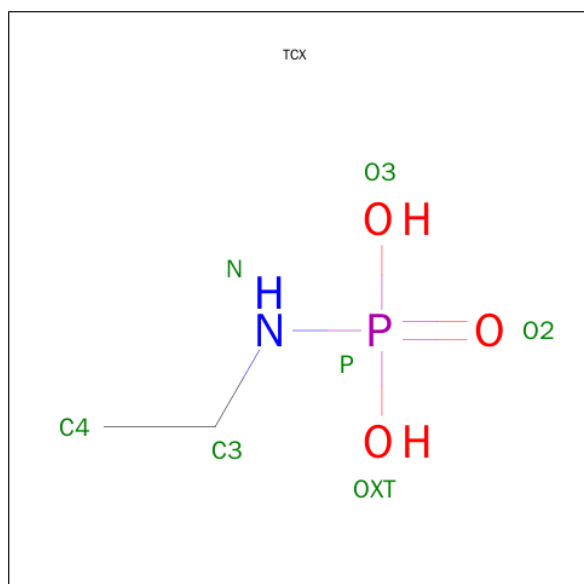
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	7	2	0
			4205	2714	707	769	15			
1	B	524	Total	C	N	O	S	0	3	0
			4192	2708	705	764	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
B	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
B	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 2 is ETHYLPHOSPHORAMIDIC ACID (three-letter code: TCX) (formula:  $C_2H_8NO_3P$ ).

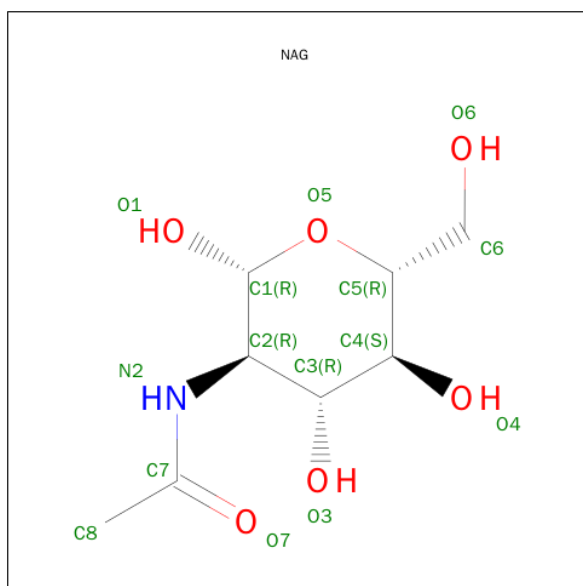


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			6	2	1	2	1		
2	B	1	Total	C	N	O	P	0	0
			6	2	1	2	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	3	Total	C	N	O		0	0
			38	22	2	14			
3	A	3	Total	C	N	O		0	0
			38	22	2	14			
3	B	3	Total	C	N	O		0	0
			38	22	2	14			
3	B	3	Total	C	N	O		0	0
			38	22	2	14			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

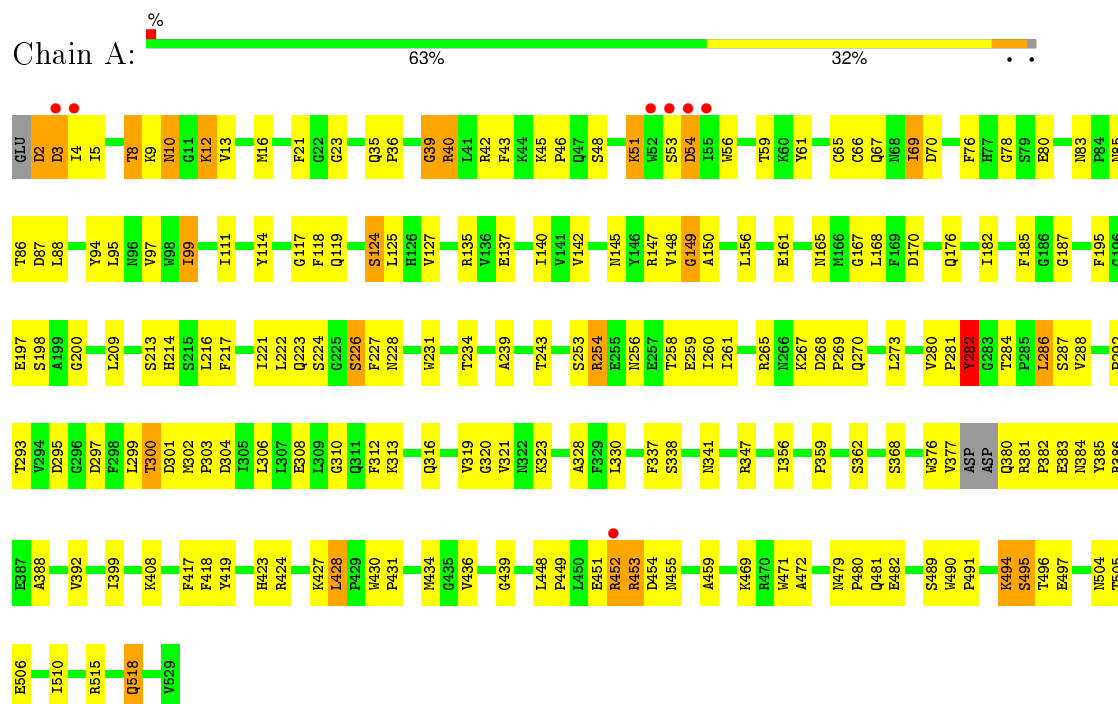
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	65	Total 65	O 65	0	0
7	B	72	Total 72	O 72	0	0

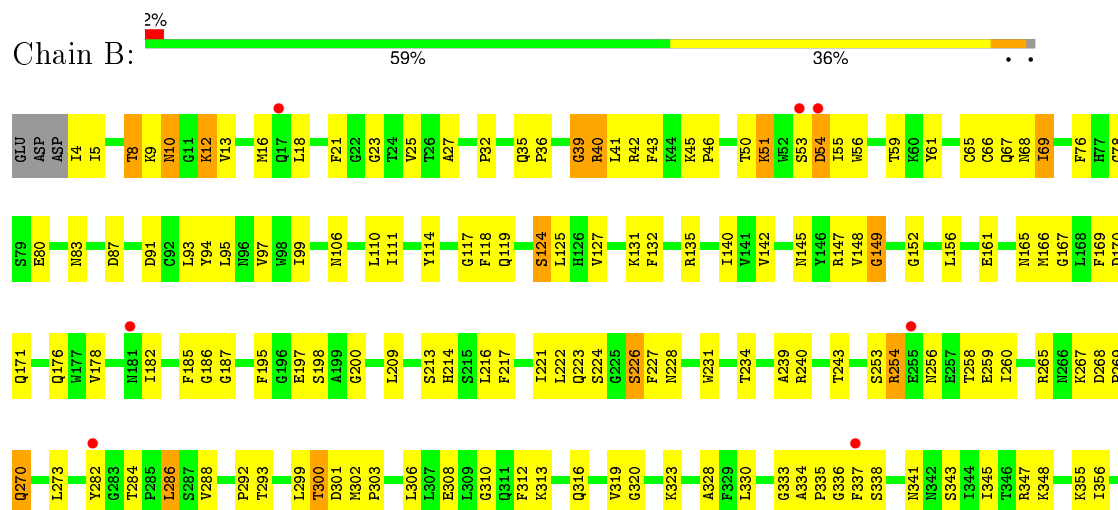
### 3 Residue-property plots

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.

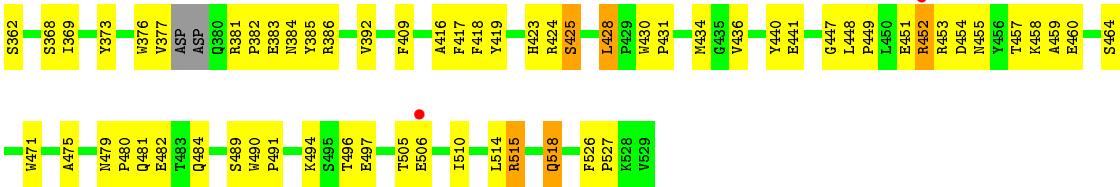
#### • Molecule 1: CHOLINESTERASE



#### • Molecule 1: CHOLINESTERASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.35Å 150.35Å 139.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 3.10 48.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.39-3.10) 98.3 (48.40-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.70 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.220 , 0.253 0.216 , 0.248	Depositor DCC
$R_{free}$ test set	937 reflections (3.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 29105 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: FUC, SO4, NAG, TCX, 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	0.63	1/4327 (0.0%)	0.69	2/5874 (0.0%)
1	B	0.59	0/4317	0.66	0/5860
All	All	0.61	1/8644 (0.0%)	0.67	2/11734 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	TYR	CB-CG	-11.40	1.34	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	TYR	CB-CG-CD1	-12.51	113.50	121.00
1	A	282	TYR	CB-CG-CD2	12.29	128.37	121.00

There are no chirality outliers.

There are no planarity outliers.

### 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	4205	0	4098	166	0
1	B	4192	0	4095	167	0
2	A	6	0	7	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	7	2	0
3	A	76	0	68	3	0
3	B	76	0	68	1	0
4	A	42	0	39	0	0
4	B	42	0	39	1	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	1	0	0	0	0
7	A	65	0	0	16	0
7	B	72	0	0	18	0
All	All	8798	0	8421	334	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 20.

All (334) 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:2:ASP:HA	1:A:3:ASP:O	1.30	1.28
1:A:253:SER:O	1:A:254:ARG:HD3	1.55	1.05
1:B:452:ARG:HA	1:B:452:ARG:HE	1.20	1.04
1:A:494:LYS:HE2	7:A:2057:HOH:O	1.58	1.02
1:A:452:ARG:HE	1:A:452:ARG:HA	1.20	1.02
1:A:518:GLN:H	1:A:518:GLN:NE2	1.59	0.99
1:B:518:GLN:NE2	1:B:518:GLN:H	1.61	0.97
1:B:4:ILE:HG12	7:B:2001:HOH:O	1.65	0.96
1:B:518:GLN:HE21	1:B:518:GLN:N	1.66	0.93
1:B:53:SER:O	1:B:54:ASP:HB2	1.69	0.91
1:B:253:SER:O	1:B:254:ARG:HD3	1.71	0.90
1:A:518:GLN:HE21	1:A:518:GLN:N	1.70	0.90
1:A:53:SER:O	1:A:54:ASP:HB2	1.72	0.88
1:A:518:GLN:H	1:A:518:GLN:HE21	0.87	0.86
1:B:40:ARG:HD2	7:B:2009:HOH:O	1.73	0.86
1:A:2:ASP:HA	1:A:3:ASP:C	1.97	0.85
1:B:156:LEU:HD13	1:B:243:THR:HG21	1.60	0.83
1:B:53:SER:O	1:B:54:ASP:CB	2.27	0.81
1:B:452:ARG:HA	1:B:452:ARG:NE	1.96	0.81
1:A:53:SER:O	1:A:54:ASP:CB	2.25	0.80
1:B:16:MET:HB3	1:B:59:THR:HG22	1.63	0.80
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.63	0.79
1:B:284:THR:HG22	1:B:356:ILE:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG12	1:A:288:VAL:O	1.83	0.77
1:A:284:THR:HG22	1:A:356:ILE:O	1.85	0.77
1:B:430:TRP:HB3	1:B:431:PRO:HD2	1.66	0.77
1:A:23:GLY:HA3	1:A:135:ARG:HE	1.50	0.76
1:B:286:LEU:HD23	2:B:600:TCX:H43C	1.67	0.76
1:B:23:GLY:HA3	1:B:135:ARG:HE	1.51	0.75
1:A:452:ARG:NE	1:A:452:ARG:HA	1.99	0.75
1:A:430:TRP:HB3	1:A:431:PRO:HD2	1.69	0.74
1:B:288:VAL:HG12	1:B:288:VAL:O	1.86	0.74
1:B:491:PRO:CD	1:B:510:ILE:HD12	2.19	0.72
1:B:161:GLU:HG3	1:B:258:THR:HG23	1.72	0.72
1:B:213:SER:HA	1:B:216:LEU:HD12	1.71	0.71
1:A:16:MET:HB3	1:A:59:THR:HG22	1.72	0.71
1:A:213:SER:HA	1:A:216:LEU:HD12	1.72	0.70
1:A:217:PHE:O	1:A:313:LYS:NZ	2.24	0.70
1:A:504:ASN:HB2	7:A:2058:HOH:O	1.91	0.70
1:B:518:GLN:HE21	1:B:518:GLN:H	0.81	0.69
1:A:2:ASP:O	1:A:2:ASP:CG	2.31	0.69
1:B:46:PRO:HD3	1:B:147:ARG:NH2	2.08	0.69
1:B:209:LEU:CD2	1:B:312:PHE:HB3	2.23	0.69
1:A:491:PRO:CD	1:A:510:ILE:HD12	2.22	0.69
1:A:2:ASP:CA	1:A:3:ASP:O	2.26	0.68
1:B:69:ILE:HA	7:B:2017:HOH:O	1.94	0.68
1:B:99:ILE:HG22	1:B:140:ILE:HG12	1.74	0.68
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.75	0.67
1:A:39:GLY:O	1:A:265:ARG:HD3	1.94	0.67
1:B:99:ILE:HG21	1:B:185:PHE:HB3	1.77	0.66
1:B:316:GLN:CD	1:B:316:GLN:H	1.98	0.66
1:A:209:LEU:CD2	1:A:312:PHE:HB3	2.26	0.66
1:B:42:ARG:HH22	1:B:269:PRO:HD3	1.61	0.66
1:B:5:ILE:HD11	7:B:2004:HOH:O	1.96	0.66
1:B:39:GLY:O	1:B:265:ARG:HD3	1.96	0.65
1:B:69:ILE:HG23	1:B:83:ASN:OD1	1.97	0.65
1:B:491:PRO:HD3	1:B:510:ILE:HD12	1.79	0.65
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.78	0.64
1:B:452:ARG:CA	1:B:452:ARG:HE	2.05	0.64
1:A:380:GLN:OE1	7:A:2041:HOH:O	2.15	0.64
1:B:221:ILE:C	1:B:222:LEU:HD12	2.18	0.64
1:B:491:PRO:HD3	1:B:510:ILE:CD1	2.27	0.63
1:B:42:ARG:NH2	1:B:269:PRO:HD3	2.13	0.63
1:A:286:LEU:HD23	2:A:600:TCX:H43C	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:PRO:HD3	1:A:510:ILE:CD1	2.29	0.62
1:B:65:CYS:O	1:B:67:GLN:HG2	1.99	0.62
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.81	0.62
1:A:3:ASP:OD2	1:A:5:ILE:HD11	2.00	0.62
1:A:65:CYS:O	1:A:67:GLN:HG2	1.99	0.62
1:A:99:ILE:HG22	1:A:140:ILE:HG12	1.83	0.61
1:A:303:PRO:HA	1:A:306:LEU:HD12	1.81	0.61
1:A:114:TYR:HE2	1:A:145:ASN:HA	1.65	0.61
1:B:454:ASP:O	1:B:455:ASN:HB2	2.00	0.61
1:A:453:ARG:HD3	7:A:2051:HOH:O	2.02	0.59
3:A:1535:NAG:H5	7:A:2063:HOH:O	2.03	0.59
1:B:491:PRO:CD	1:B:510:ILE:CD1	2.80	0.59
1:A:99:ILE:HG21	1:A:185:PHE:HB3	1.85	0.59
1:A:321:VAL:HG21	1:A:399:ILE:HG12	1.85	0.59
1:A:2:ASP:O	1:A:2:ASP:OD2	2.21	0.58
1:A:491:PRO:HD3	1:A:510:ILE:HD12	1.84	0.58
1:A:454:ASP:O	1:A:455:ASN:HB2	2.03	0.58
1:A:45:LYS:HE3	7:A:2005:HOH:O	2.04	0.58
1:A:491:PRO:CD	1:A:510:ILE:CD1	2.82	0.58
1:B:97:VAL:HG22	1:B:142:VAL:HG22	1.86	0.57
1:A:359:PRO:HD2	7:A:2038:HOH:O	2.04	0.57
1:A:119:GLN:HE22	1:A:149:GLY:HA2	1.69	0.57
1:B:95:LEU:C	1:B:95:LEU:HD12	2.25	0.57
1:A:491:PRO:HG3	1:A:510:ILE:HD12	1.87	0.57
1:A:46:PRO:HD3	1:A:147:ARG:NH2	2.20	0.57
1:B:165:ASN:OD1	1:B:292:PRO:HA	2.05	0.57
1:A:254:ARG:HB2	1:A:260:ILE:HG12	1.85	0.56
1:A:221:ILE:C	1:A:222:LEU:HD12	2.26	0.56
1:B:114:TYR:HE2	1:B:145:ASN:HA	1.69	0.56
1:A:99:ILE:HD11	7:A:2002:HOH:O	2.06	0.56
1:A:213:SER:O	1:A:214[A]:HIS:C	2.42	0.56
1:B:312:PHE:CD1	1:B:409:PHE:CE1	2.94	0.55
1:B:319:VAL:O	1:B:418:PHE:HA	2.06	0.55
1:B:226:SER:HB2	1:B:228:ASN:OD1	2.05	0.55
1:A:268[B]:ASP:OD2	1:A:270:GLN:HB2	2.07	0.55
1:A:308:GLU:HA	1:A:308:GLU:OE2	2.07	0.55
1:B:140:ILE:HG21	1:B:182:ILE:HD11	1.89	0.54
1:A:8:THR:C	1:A:10:ASN:H	2.11	0.54
1:B:312:PHE:CE1	1:B:409:PHE:CE1	2.95	0.54
1:B:32:PRO:HB3	1:B:94:TYR:CE2	2.43	0.54
1:B:76:PHE:CE2	1:B:78:GLY:HA3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:HG12	1:B:56:TRP:HB3	1.90	0.54
1:B:46:PRO:HD3	1:B:147:ARG:HH22	1.70	0.54
1:B:355:LYS:O	7:B:2047:HOH:O	2.18	0.54
1:B:8:THR:C	1:B:10:ASN:H	2.11	0.54
1:B:114:TYR:HB2	7:B:2022:HOH:O	2.07	0.54
1:A:99:ILE:CD1	7:A:2002:HOH:O	2.56	0.53
1:B:338:SER:HB3	1:B:341:ASN:OD1	2.08	0.53
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.23	0.53
1:A:491:PRO:CG	1:A:510:ILE:HD12	2.39	0.53
1:A:316:GLN:CD	1:A:316:GLN:H	2.11	0.53
1:B:383:GLU:H	1:B:383:GLU:CD	2.12	0.53
1:B:223:GLN:NE2	1:B:441:GLU:OE2	2.42	0.53
1:B:316:GLN:N	1:B:316:GLN:CD	2.63	0.53
1:B:369:ILE:HD11	1:B:526:PHE:CE1	2.44	0.52
1:B:214[A]:HIS:O	1:B:313:LYS:HE3	2.09	0.52
1:B:178:VAL:HG13	1:B:182:ILE:HB	1.90	0.52
1:A:295:ASP:OD2	1:A:297:ASP:HB3	2.09	0.52
1:B:95:LEU:O	1:B:95:LEU:HD12	2.09	0.52
1:B:197:GLU:O	1:B:200:GLY:N	2.43	0.52
1:B:310:GLY:HA2	1:B:312:PHE:CE2	2.44	0.51
1:B:231:TRP:CE2	2:B:600:TCX:H32C	2.44	0.51
1:A:42:ARG:O	1:A:43:PHE:HB2	2.10	0.51
1:B:254:ARG:HB2	1:B:260:ILE:HG12	1.92	0.51
1:A:423:HIS:ND1	1:A:505:THR:HG23	2.25	0.51
1:B:491:PRO:HG3	1:B:510:ILE:HD12	1.93	0.50
1:A:383:GLU:H	1:A:383:GLU:CD	2.13	0.50
1:A:12:LYS:HE2	7:A:2001:HOH:O	2.11	0.50
1:B:106:ASN:ND2	4:B:1537:NAG:C7	2.75	0.50
1:B:10:ASN:HD22	1:B:51:LYS:HA	1.76	0.50
1:A:161:GLU:OE1	1:A:161:GLU:HA	2.12	0.50
1:B:303:PRO:HD2	7:B:2043:HOH:O	2.10	0.49
1:B:491:PRO:CG	1:B:510:ILE:HD12	2.42	0.49
1:A:80:GLU:HG2	7:A:2011:HOH:O	2.13	0.49
1:A:452:ARG:HE	1:A:452:ARG:CA	2.05	0.49
1:A:423:HIS:CE1	1:A:505:THR:CG2	2.95	0.49
1:B:320:GLY:HA3	1:B:419:TYR:CD1	2.47	0.49
1:A:319:VAL:O	1:A:418:PHE:HA	2.13	0.49
1:B:42:ARG:O	1:B:43:PHE:HB2	2.13	0.49
1:A:337:PHE:HE2	1:A:386:ARG:HG3	1.76	0.49
1:B:213:SER:O	1:B:214[A]:HIS:C	2.50	0.49
1:B:119:GLN:NE2	1:B:149:GLY:HA2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:SER:HB2	3:A:1534:NAG:H62	1.94	0.49
1:B:167:GLY:O	1:B:170:ASP:HB2	2.12	0.49
1:A:119:GLN:NE2	1:A:149:GLY:HA2	2.27	0.49
1:A:69:ILE:HG23	1:A:83:ASN:OD1	2.13	0.49
1:B:320:GLY:HA3	1:B:419:TYR:CE1	2.47	0.49
1:A:95:LEU:HD12	1:A:95:LEU:C	2.33	0.49
1:B:301:ASP:OD2	1:B:302:MET:N	2.45	0.49
1:A:388:ALA:O	1:A:392:VAL:HG23	2.12	0.49
1:A:5:ILE:HD12	1:A:5:ILE:N	2.28	0.49
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.48	0.49
1:B:140:ILE:HD12	1:B:187:GLY:HA2	1.94	0.48
1:A:376:TRP:CE3	1:A:376:TRP:HA	2.48	0.48
1:B:214[B]:HIS:O	1:B:313:LYS:HE3	2.13	0.48
1:B:288:VAL:CG1	1:B:288:VAL:O	2.57	0.48
1:A:167:GLY:O	1:A:170:ASP:HB2	2.13	0.48
1:B:447:GLY:HA2	1:B:464:SER:OG	2.14	0.48
1:B:66:CYS:HB3	1:B:273:LEU:HD11	1.95	0.48
1:A:8:THR:C	1:A:10:ASN:N	2.67	0.48
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.49	0.48
1:A:518:GLN:NE2	1:A:518:GLN:N	2.43	0.48
1:A:66:CYS:HB3	1:A:273:LEU:HD11	1.96	0.48
1:B:217:PHE:O	1:B:313:LYS:NZ	2.37	0.48
1:A:114:TYR:CE2	1:A:145:ASN:HA	2.48	0.48
1:B:376:TRP:HA	1:B:376:TRP:CE3	2.48	0.48
1:A:231:TRP:CE2	2:A:600:TCX:H32C	2.49	0.48
1:A:95:LEU:HD12	1:A:95:LEU:O	2.14	0.48
1:B:300:THR:O	1:B:301:ASP:HB2	2.13	0.47
1:B:4:ILE:HG22	7:B:2005:HOH:O	2.14	0.47
1:B:50:THR:HA	7:B:2011:HOH:O	2.15	0.47
1:A:85:ASN:O	1:A:86:THR:HG22	2.13	0.47
1:B:80:GLU:HA	1:B:83:ASN:HD22	1.77	0.47
1:B:35:GLN:O	1:B:36:PRO:C	2.52	0.47
1:B:209:LEU:HD11	1:B:227:PHE:CE1	2.49	0.47
1:A:140:ILE:HD12	1:A:187:GLY:HA2	1.96	0.47
1:A:70:ASP:C	1:A:70:ASP:OD2	2.51	0.47
1:A:140:ILE:HG21	1:A:182:ILE:HD11	1.96	0.47
1:B:459:ALA:HB1	1:B:505:THR:HB	1.96	0.47
1:A:284:THR:H	1:A:287:SER:HG	1.54	0.47
1:A:491:PRO:HD3	1:A:510:ILE:HD11	1.96	0.47
1:A:380:GLN:N	7:A:2041:HOH:O	2.46	0.47
1:B:303:PRO:HA	1:B:306:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLN:HE22	1:B:149:GLY:HA2	1.78	0.47
1:A:495:SER:HB3	7:A:2045:HOH:O	2.14	0.47
1:A:80:GLU:HA	1:A:83:ASN:HD22	1.79	0.47
1:A:97:VAL:HG22	1:A:142:VAL:HG22	1.95	0.47
1:B:110:LEU:HD11	1:B:475:ALA:CB	2.45	0.47
1:B:312:PHE:CE1	1:B:409:PHE:CD1	3.04	0.46
1:A:80:GLU:HA	1:A:83:ASN:ND2	2.31	0.46
1:A:119:GLN:O	1:A:148:VAL:HG21	2.16	0.46
1:A:299:LEU:HA	1:A:299:LEU:HD23	1.74	0.46
1:B:416:ALA:N	7:B:2052:HOH:O	2.47	0.46
1:B:417:PHE:HB3	1:B:490:TRP:CE2	2.51	0.46
1:B:8:THR:C	1:B:10:ASN:N	2.69	0.46
1:B:381:ARG:NH2	1:B:383:GLU:OE1	2.49	0.46
1:A:423:HIS:CE1	1:A:505:THR:HG21	2.50	0.46
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.31	0.45
1:B:152:GLY:O	1:B:166:MET:HB2	2.16	0.45
1:B:268[B]:ASP:OD2	1:B:270:GLN:HB2	2.16	0.45
1:B:51:LYS:NZ	7:B:2011:HOH:O	2.50	0.45
1:A:197:GLU:O	1:A:200:GLY:N	2.44	0.45
1:B:514:LEU:O	1:B:515:ARG:C	2.53	0.45
1:B:328:ALA:HA	1:B:434:MET:CE	2.47	0.45
1:B:13:VAL:HA	1:B:56:TRP:O	2.16	0.45
1:B:167:GLY:O	1:B:171:GLN:HG3	2.17	0.45
1:A:137:GLU:OE2	1:A:469:LYS:HE2	2.16	0.45
1:B:308:GLU:OE2	1:B:308:GLU:HA	2.16	0.45
1:A:424:ARG:HH12	1:A:428:LEU:HD12	1.81	0.45
1:A:280:VAL:HB	1:A:281:PRO:HD2	1.97	0.45
1:B:518:GLN:NE2	1:B:518:GLN:N	2.43	0.45
1:B:334:ALA:HB3	1:B:337:PHE:CD1	2.52	0.45
1:B:234:THR:O	1:B:293:THR:HG22	2.16	0.45
1:B:479:ASN:OD1	1:B:481:GLN:HG2	2.16	0.45
1:B:50:THR:O	1:B:51:LYS:C	2.54	0.45
1:B:337:PHE:HE2	1:B:386:ARG:HG3	1.81	0.44
1:B:341:ASN:ND2	3:B:1534:NAG:O7	2.49	0.44
1:A:40:ARG:HG2	7:A:2003:HOH:O	2.16	0.44
1:B:381:ARG:HA	1:B:382:PRO:HD3	1.77	0.44
1:B:68:ASN:OD1	1:B:273:LEU:HB3	2.18	0.44
1:A:376:TRP:HA	1:A:376:TRP:HE3	1.83	0.44
1:B:491:PRO:HD3	1:B:510:ILE:HD11	2.00	0.44
1:A:338:SER:HB3	1:A:341:ASN:OD1	2.17	0.44
1:B:186:GLY:O	7:B:2027:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TYR:CG	1:B:124:SER:HB3	2.53	0.44
1:B:424:ARG:NH1	1:B:428:LEU:HD12	2.32	0.44
1:A:165:ASN:OD1	1:A:292:PRO:HA	2.17	0.44
1:A:424:ARG:NH2	1:A:430:TRP:O	2.49	0.44
1:B:383:GLU:O	1:B:384:ASN:C	2.57	0.44
1:B:282:TYR:HB3	7:B:2037:HOH:O	2.17	0.44
1:B:348:LYS:HB2	7:B:2046:HOH:O	2.16	0.44
1:B:239:ALA:HB2	1:B:293:THR:HG21	2.00	0.44
1:B:448:LEU:N	1:B:449:PRO:CD	2.81	0.44
1:A:197:GLU:OE2	1:A:439:GLY:HA2	2.18	0.43
1:A:21:PHE:HE2	1:A:451:GLU:HA	1.83	0.43
1:B:65:CYS:HB3	7:B:2016:HOH:O	2.17	0.43
1:B:213:SER:HA	1:B:216:LEU:CD1	2.43	0.43
1:B:111:ILE:HA	1:B:142:VAL:O	2.19	0.43
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.83	0.43
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.54	0.43
1:A:304:ASP:OD1	1:A:304:ASP:N	2.50	0.43
1:B:515:ARG:NE	7:B:2068:HOH:O	2.51	0.43
1:A:137:GLU:HG3	1:A:472:ALA:HB2	2.01	0.43
1:B:333:GLY:O	1:B:335:PRO:HD3	2.18	0.43
1:B:440:TYR:HA	7:B:2055:HOH:O	2.19	0.43
1:A:341:ASN:ND2	3:A:1534:NAG:O7	2.51	0.43
1:A:4:ILE:O	1:A:4:ILE:HG23	2.19	0.43
1:B:376:TRP:HA	1:B:376:TRP:HE3	1.83	0.43
1:A:119:GLN:O	1:A:148:VAL:CG2	2.67	0.43
1:A:316:GLN:CD	1:A:316:GLN:N	2.72	0.43
1:A:239:ALA:HB2	1:A:293:THR:HG21	2.01	0.43
1:B:12:LYS:HB2	1:B:55:ILE:HG12	2.00	0.43
1:B:21:PHE:HE2	1:B:451:GLU:HA	1.84	0.43
1:A:459:ALA:HB1	1:A:505:THR:HB	2.01	0.42
1:A:280:VAL:HG23	1:A:282:TYR:O	2.19	0.42
1:A:234:THR:HB	1:A:293:THR:HG22	2.01	0.42
1:A:328:ALA:HA	1:A:434:MET:CE	2.49	0.42
1:A:448:LEU:N	1:A:449:PRO:CD	2.82	0.42
1:A:2:ASP:CA	1:A:3:ASP:C	2.76	0.42
1:A:337:PHE:CE2	1:A:386:ARG:HG3	2.53	0.42
1:B:423:HIS:ND1	1:B:505:THR:HG23	2.34	0.42
1:A:227:PHE:C	1:A:227:PHE:CD2	2.93	0.42
1:B:459:ALA:HA	7:B:2059:HOH:O	2.19	0.42
1:B:457:THR:OG1	1:B:460:GLU:HG3	2.20	0.42
1:A:300:THR:O	1:A:301:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:HIS:CE1	1:A:505:THR:HG23	2.54	0.42
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.68	0.42
1:A:118:PHE:O	1:A:148:VAL:HB	2.20	0.42
1:A:149:GLY:O	1:A:150:ALA:C	2.57	0.42
1:A:10:ASN:HD22	1:A:51:LYS:HA	1.85	0.42
1:A:427:LYS:HE3	1:A:427:LYS:HB3	1.88	0.42
1:B:256:ASN:O	1:B:259:GLU:HB2	2.20	0.42
1:B:373:TYR:CD2	1:B:392:VAL:HG22	2.55	0.42
1:A:256:ASN:O	1:A:259:GLU:HB2	2.20	0.42
1:B:234:THR:HB	1:B:293:THR:CG2	2.50	0.42
1:B:425:SER:O	1:B:428:LEU:HB2	2.20	0.42
1:B:484:GLN:HB2	1:B:484:GLN:HE21	1.62	0.42
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.82	0.42
1:A:214[A]:HIS:HE1	7:A:2022:HOH:O	2.02	0.42
1:A:376:TRP:HH2	1:A:388:ALA:HB2	1.85	0.42
1:A:408:LYS:HB3	7:A:2044:HOH:O	2.20	0.42
1:A:13:VAL:HA	1:A:56:TRP:O	2.20	0.42
1:B:185:PHE:CD1	1:B:185:PHE:N	2.87	0.42
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.75	0.42
1:B:526:PHE:N	1:B:527:PRO:CD	2.83	0.41
1:B:45:LYS:HD3	1:B:169:PHE:CE1	2.55	0.41
1:A:76:PHE:CE2	1:A:78:GLY:HA3	2.55	0.41
1:B:336:GLY:HA3	1:B:345:ILE:HG22	2.02	0.41
1:A:99:ILE:O	1:A:99:ILE:HG13	2.19	0.41
1:B:347:ARG:HB2	1:B:385:TYR:CZ	2.55	0.41
1:A:209:LEU:HD11	1:A:227:PHE:CE1	2.55	0.41
1:A:198:SER:HA	1:A:224:SER:O	2.21	0.41
1:B:18:LEU:HD11	1:B:27:ALA:HB2	2.01	0.41
1:A:111:ILE:HA	1:A:142:VAL:O	2.20	0.41
1:B:480:PRO:HB2	1:B:490:TRP:CE3	2.54	0.41
1:B:337:PHE:HA	1:B:343:SER:OG	2.20	0.41
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.54	0.41
1:A:383:GLU:O	1:A:384:ASN:C	2.59	0.41
1:A:234:THR:O	1:A:293:THR:HG22	2.20	0.41
1:A:479:ASN:OD1	1:A:481:GLN:HG2	2.21	0.41
1:A:480:PRO:HB2	1:A:490:TRP:CE3	2.55	0.41
1:B:131:LYS:HE2	1:B:132:PHE:CZ	2.55	0.41
1:B:91:ASP:OD1	1:B:91:ASP:C	2.59	0.41
1:A:35:GLN:O	1:A:36:PRO:C	2.58	0.41
1:A:156:LEU:HD22	1:A:261:ILE:HD11	2.03	0.41
1:A:227:PHE:CD2	1:A:228:ASN:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:HIS:CE1	1:B:505:THR:CG2	3.03	0.41
1:A:88:LEU:HD23	1:A:88:LEU:N	2.34	0.41
1:A:226:SER:HB2	1:A:228:ASN:OD1	2.21	0.41
1:B:93:LEU:HD23	1:B:93:LEU:N	2.34	0.41
1:A:381:ARG:HA	1:A:382:PRO:HD3	1.78	0.41
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.89	0.41
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.93	0.41
1:A:197:GLU:HA	1:A:223:GLN:O	2.21	0.41
1:A:301:ASP:OD2	1:A:302:MET:N	2.54	0.41
1:A:13:VAL:HG12	1:A:56:TRP:HB3	2.02	0.41
1:B:25:VAL:HG13	1:B:99:ILE:O	2.21	0.40
1:A:268[B]:ASP:OD2	1:A:270:GLN:CB	2.68	0.40
1:A:61:TYR:CG	1:A:124:SER:HB3	2.56	0.40
1:B:5:ILE:N	1:B:5:ILE:HD12	2.35	0.40
1:A:417:PHE:HB3	1:A:490:TRP:CE2	2.56	0.40
1:A:94:TYR:N	1:A:94:TYR:CD1	2.89	0.40
1:B:458:LYS:HD2	1:B:458:LYS:HA	1.76	0.40
1:B:4:ILE:O	1:B:4:ILE:HG23	2.21	0.40
1:A:231:TRP:CD2	2:A:600:TCX:H32C	2.56	0.40
1:B:118:PHE:O	1:B:148:VAL:HB	2.22	0.40
1:B:76:PHE:O	1:B:80:GLU:HB2	2.21	0.40
1:A:168:LEU:HA	1:A:168:LEU:HD23	1.80	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	524/529 (99%)	465 (89%)	49 (9%)	10 (2%)	10	40
1	B	523/529 (99%)	466 (89%)	47 (9%)	10 (2%)	10	40
All	All	1047/1058 (99%)	931 (89%)	96 (9%)	20 (2%)	10	40

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	54	ASP
1	B	54	ASP
1	A	39	GLY
1	A	149	GLY
1	A	362	SER
1	A	506	GLU
1	B	39	GLY
1	B	362	SER
1	B	453	ARG
1	B	506	GLU
1	B	224	SER
1	A	9	LYS
1	A	453	ARG
1	B	9	LYS
1	B	436	VAL
1	A	117	GLY
1	A	436	VAL
1	B	117	GLY
1	B	149	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	452/454 (100%)	417 (92%)	35 (8%)	16	50
1	B	451/454 (99%)	417 (92%)	34 (8%)	17	51
All	All	903/908 (99%)	834 (92%)	69 (8%)	16	51

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	8	THR
1	A	10	ASN

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Mol	Chain	Res	Type
1	A	12	LYS
1	A	40	ARG
1	A	48	SER
1	A	51	LYS
1	A	69	ILE
1	A	87	ASP
1	A	99	ILE
1	A	124	SER
1	A	125	LEU
1	A	127	VAL
1	A	176	GLN
1	A	195	PHE
1	A	226	SER
1	A	254	ARG
1	A	267	LYS
1	A	282	TYR
1	A	286	LEU
1	A	300	THR
1	A	323	LYS
1	A	368	SER
1	A	377	VAL
1	A	428	LEU
1	A	452	ARG
1	A	471	TRP
1	A	482	GLU
1	A	489	SER
1	A	494	LYS
1	A	495	SER
1	A	496	THR
1	A	497	GLU
1	A	515	ARG
1	A	518	GLN
1	B	8	THR
1	B	10	ASN
1	B	12	LYS
1	B	40	ARG
1	B	51	LYS
1	B	69	ILE
1	B	87	ASP
1	B	124	SER
1	B	125	LEU
1	B	127	VAL

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Mol	Chain	Res	Type
1	B	176	GLN
1	B	195	PHE
1	B	198	SER
1	B	226	SER
1	B	240	ARG
1	B	254	ARG
1	B	267	LYS
1	B	270	GLN
1	B	286	LEU
1	B	300	THR
1	B	323	LYS
1	B	368	SER
1	B	377	VAL
1	B	425	SER
1	B	428	LEU
1	B	452	ARG
1	B	471	TRP
1	B	482	GLU
1	B	489	SER
1	B	494	LYS
1	B	496	THR
1	B	497	GLU
1	B	515	ARG
1	B	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	17	GLN
1	A	71	GLN
1	A	119	GLN
1	A	172	GLN
1	A	322	ASN
1	A	372	HIS
1	A	484	GLN
1	A	518	GLN
1	B	10	ASN
1	B	17	GLN
1	B	71	GLN
1	B	119	GLN
1	B	172	GLN

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Mol	Chain	Res	Type
1	B	322	ASN
1	B	372	HIS
1	B	484	GLN
1	B	518	GLN

### 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 ⓘ

12 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	A	1531	1,3	14,14,15	0.54	0	15,19,21	1.68	2 (13%)
3	NAG	A	1532	3	14,14,15	0.42	0	15,19,21	1.72	2 (13%)
3	FUC	A	1533	3	10,10,11	0.55	0	14,14,16	1.03	1 (7%)
3	NAG	A	1534	1,3	14,14,15	0.66	0	15,19,21	0.68	0
3	NAG	A	1535	3	14,14,15	0.42	0	15,19,21	2.29	5 (33%)
3	FUC	A	1536	3	10,10,11	0.60	0	14,14,16	1.60	4 (28%)
3	NAG	B	1531	1,3	14,14,15	0.61	0	15,19,21	1.94	2 (13%)
3	NAG	B	1532	3	14,14,15	0.47	0	15,19,21	1.64	1 (6%)
3	FUC	B	1533	3	10,10,11	0.64	0	14,14,16	1.06	1 (7%)
3	NAG	B	1534	1,3	14,14,15	0.57	0	15,19,21	0.79	0
3	NAG	B	1535	3	14,14,15	0.43	0	15,19,21	2.40	4 (26%)
3	FUC	B	1536	3	10,10,11	0.65	0	14,14,16	1.69	3 (21%)



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	A	1531	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1532	3	-	0/6/23/26	0/1/1/1
3	FUC	A	1533	3	-	0/0/17/20	0/1/1/1
3	NAG	A	1534	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1535	3	-	0/6/23/26	0/1/1/1
3	FUC	A	1536	3	-	0/0/17/20	0/1/1/1
3	NAG	B	1531	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1532	3	-	0/6/23/26	0/1/1/1
3	FUC	B	1533	3	-	0/0/17/20	0/1/1/1
3	NAG	B	1534	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1535	3	-	0/6/23/26	0/1/1/1
3	FUC	B	1536	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1536	FUC	C1-C2-C3	-4.05	104.75	109.54
3	B	1535	NAG	C6-C5-C4	-3.85	103.51	113.02
3	A	1535	NAG	C4-C3-C2	-3.14	106.36	111.23
3	A	1536	FUC	C1-C2-C3	-3.09	105.88	109.54
3	B	1535	NAG	C4-C3-C2	-3.07	106.46	111.23
3	A	1535	NAG	C6-C5-C4	-2.90	105.86	113.02
3	A	1535	NAG	C2-N2-C7	-2.30	120.08	123.04
3	A	1532	NAG	C2-N2-C7	-2.22	120.18	123.04
3	A	1535	NAG	C3-C4-C5	2.04	113.76	110.20
3	A	1536	FUC	O5-C5-C4	2.07	113.12	109.53
3	B	1533	FUC	C1-C2-C3	2.10	112.03	109.54
3	A	1533	FUC	C3-C4-C5	2.15	113.34	109.72
3	A	1536	FUC	O5-C5-C6	2.21	109.78	106.13
3	B	1535	NAG	C3-C4-C5	2.57	114.68	110.20
3	B	1536	FUC	O5-C5-C6	2.68	110.56	106.13
3	B	1536	FUC	C1-O5-C5	2.80	116.70	112.38
3	A	1536	FUC	C1-O5-C5	2.97	116.96	112.38
3	A	1531	NAG	C1-O5-C5	3.41	116.57	112.25
3	B	1531	NAG	C4-C3-C2	4.15	117.69	111.23
3	A	1531	NAG	C4-C3-C2	4.25	117.84	111.23
3	B	1531	NAG	C1-O5-C5	4.95	118.53	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1532	NAG	C1-O5-C5	5.20	118.85	112.25
3	A	1532	NAG	C1-O5-C5	5.32	119.00	112.25
3	A	1535	NAG	C1-O5-C5	6.59	120.61	112.25
3	B	1535	NAG	C1-O5-C5	6.86	120.95	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1534	NAG	2	0
3	A	1535	NAG	1	0
3	B	1534	NAG	1	0

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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	$\# Z  > 2$
4	NAG	A	1537	1	14,14,15	0.57	0	15,19,21	1.97	3 (20%)
4	NAG	A	1538	1	14,14,15	0.74	1 (7%)	15,19,21	1.88	3 (20%)
4	NAG	A	1539	1	14,14,15	0.53	0	15,19,21	0.75	0
5	SO4	A	1540	-	4,4,4	0.18	0	6,6,6	0.26	0
5	SO4	A	1541	-	4,4,4	0.17	0	6,6,6	0.21	0
2	TCX	A	600	1	2,5,6	0.63	0	1,5,8	1.48	0
4	NAG	B	1537	1	14,14,15	0.69	0	15,19,21	1.84	3 (20%)
4	NAG	B	1538	1	14,14,15	0.48	0	15,19,21	1.78	3 (20%)
4	NAG	B	1539	1	14,14,15	0.50	0	15,19,21	0.97	1 (6%)
5	SO4	B	1540	-	4,4,4	0.15	0	6,6,6	0.18	0
2	TCX	B	600	1	2,5,6	0.57	0	1,5,8	1.04	0

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
4	NAG	A	1537	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1538	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1539	1	-	0/6/23/26	0/1/1/1
5	SO4	A	1540	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1541	-	-	0/0/0/0	0/0/0/0
2	TCX	A	600	1	-	0/0/3/4	0/0/0/0
4	NAG	B	1537	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1538	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1539	1	-	0/6/23/26	0/1/1/1
5	SO4	B	1540	-	-	0/0/0/0	0/0/0/0
2	TCX	B	600	1	-	0/0/3/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1538	NAG	C1-C2	2.18	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1538	NAG	C2-N2-C7	-4.84	116.81	123.04
4	A	1537	NAG	C2-N2-C7	-4.52	117.23	123.04
4	B	1537	NAG	C2-N2-C7	-4.26	117.56	123.04
4	B	1538	NAG	C2-N2-C7	-4.18	117.67	123.04
4	B	1537	NAG	C4-C3-C2	-3.96	105.08	111.23
4	A	1537	NAG	C4-C3-C2	-3.00	106.56	111.23
4	B	1539	NAG	C2-N2-C7	-2.71	119.56	123.04
4	B	1538	NAG	C3-C4-C5	2.73	114.96	110.20
4	A	1538	NAG	C3-C4-C5	2.74	114.97	110.20
4	B	1537	NAG	C1-O5-C5	2.90	115.93	112.25
4	A	1538	NAG	C1-O5-C5	4.21	117.60	112.25
4	B	1538	NAG	C1-O5-C5	4.32	117.73	112.25
4	A	1537	NAG	C1-O5-C5	4.85	118.40	112.25

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1537	NAG	C8-C7-N2-C2
4	B	1538	NAG	O7-C7-N2-C2
4	A	1538	NAG	O7-C7-N2-C2
4	A	1538	NAG	C8-C7-N2-C2
4	A	1537	NAG	O7-C7-N2-C2
4	A	1537	NAG	C8-C7-N2-C2
4	B	1537	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	TCX	3	0
4	B	1537	NAG	1	0
2	B	600	TCX	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	526/529 (99%)	-0.03	7 (1%) 79 62	53, 71, 95, 107	4 (0%)
1	B	524/529 (99%)	-0.06	9 (1%) 73 52	53, 71, 95, 106	3 (0%)
All	All	1050/1058 (99%)	-0.04	16 (1%) 76 58	53, 71, 95, 107	7 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	SER	3.3
1	A	53	SER	3.3
1	A	54	ASP	3.3
1	A	3	ASP	3.2
1	B	17	GLN	3.0
1	B	452	ARG	3.0
1	B	255	GLU	2.8
1	A	55	ILE	2.6
1	A	452	ARG	2.5
1	B	337	PHE	2.4
1	B	282	TYR	2.4
1	B	506	GLU	2.4
1	B	54	ASP	2.4
1	A	52	TRP	2.3
1	A	4	ILE	2.3
1	B	181	ASN	2.3

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

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

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FUC	A	1533	10/11	0.86	0.53	3.37	115,116,116,117	0
3	FUC	B	1533	10/11	0.87	0.46	2.44	114,115,115,116	0
3	FUC	A	1536	10/11	0.90	0.32	-	106,107,108,108	0
3	NAG	B	1535	14/15	0.78	0.36	-	106,108,110,111	0
3	NAG	A	1535	14/15	0.79	0.28	-	106,109,111,112	0
3	NAG	B	1532	14/15	0.74	0.33	-	123,125,126,127	0
3	NAG	B	1531	14/15	0.91	0.25	-	108,114,116,119	0
3	NAG	A	1531	14/15	0.80	0.35	-	109,115,117,121	0
3	FUC	B	1536	10/11	0.88	0.31	-	105,107,107,108	0
3	NAG	A	1532	14/15	0.79	0.55	-	124,126,128,128	0
3	NAG	B	1534	14/15	0.91	0.26	-	91,96,101,103	0
3	NAG	A	1534	14/15	0.93	0.18	-	92,96,102,104	0

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	1539	14/15	0.84	0.28	2.41	98,102,105,106	0
2	TCX	B	600	6/7	0.96	0.22	1.20	53,54,54,55	0
2	TCX	A	600	6/7	0.98	0.26	1.11	53,54,54,54	0
5	SO4	A	1541	5/5	0.87	0.25	0.47	137,138,138,138	0
4	NAG	A	1538	14/15	0.67	0.33	-	104,105,106,106	0
5	SO4	B	1540	5/5	0.84	0.30	-	112,113,113,113	0
5	SO4	A	1540	5/5	0.92	0.21	-	105,106,106,107	0
4	NAG	A	1537	14/15	0.83	0.24	-	91,94,95,96	0
4	NAG	B	1537	14/15	0.65	0.32	-	91,94,95,96	0
6	CL	A	1542	1/1	0.88	0.20	-	70,70,70,70	0
4	NAG	B	1539	14/15	0.84	0.22	-	97,102,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1538	14/15	0.83	0.34	-	103,105,106,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.