



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 05:59 PM EDT

PDB ID : 1KYA  
Title : ACTIVE LACCASE FROM TRAMETES VERSICOLOR COMPLEXED WITH 2,5-XYLIDINE  
Authors : Bertrand, T.; Jolival, C.; Briozzo, P.; Caminade, E.; Joly, N.; Madzak, C.; Mougine, C.  
Deposited on : 2002-02-04  
Resolution : 2.40 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.35

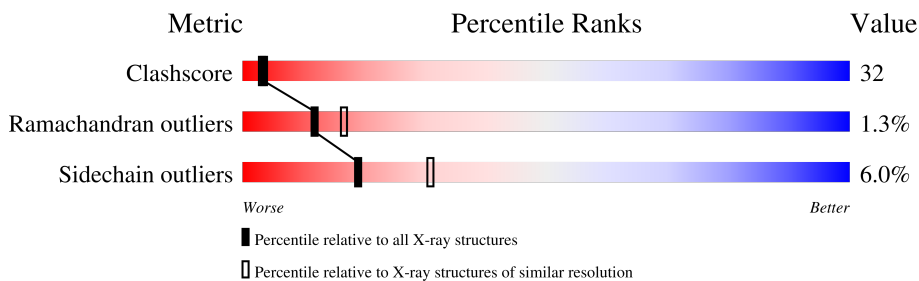
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	499	
1	B	499	
1	C	499	
1	D	499	

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	A	505	-	-	X	-
2	NAG	A	506	-	-	X	-
2	NAG	A	512	-	-	X	-
2	NAG	B	605	-	-	X	-
2	NAG	B	606	-	-	X	-
2	NAG	C	706	-	-	X	-
2	NAG	C	707	-	-	X	-
2	NAG	D	805	-	-	X	-
2	NAG	D	806	-	-	X	-
4	PYE	A	508	-	-	X	-
4	PYE	B	608	-	-	X	-
4	PYE	B	614	-	-	X	-
4	PYE	B	616	-	-	X	-
4	PYE	D	808	-	-	X	-
4	PYE	D	810	-	-	X	-
5	XYD	B	612	-	X	-	-
5	XYD	C	712	-	X	-	-

## 2 Entry composition [i](#)

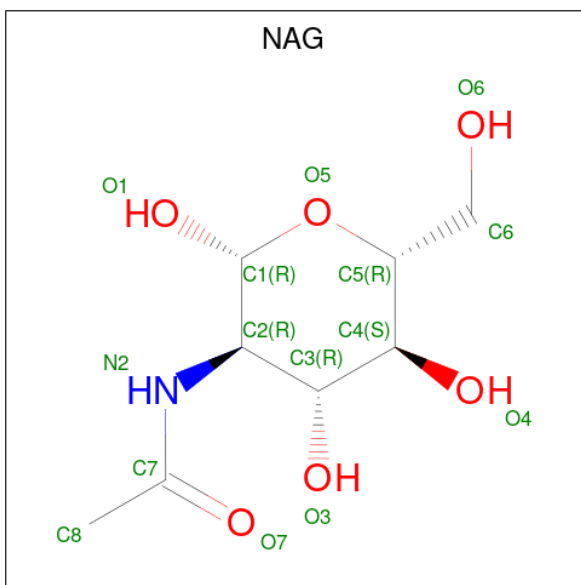
There are 6 unique types of molecules in this entry. The entry contains 16286 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LACCASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	499	Total 3753	C 2389	N 633	O 722	S 9	0	0	0
1	B	499	Total 3753	C 2389	N 633	O 722	S 9	0	0	0
1	C	499	Total 3753	C 2389	N 633	O 722	S 9	0	0	0
1	D	499	Total 3753	C 2389	N 633	O 722	S 9	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

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

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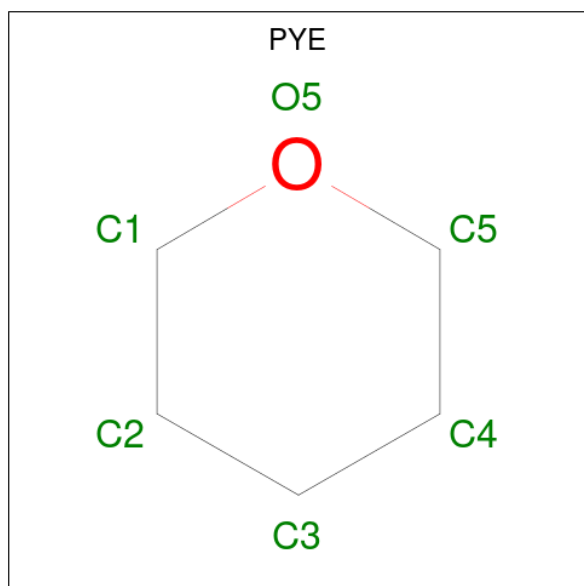
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cu	0	0
			4	4		
3	B	4	Total	Cu	0	0
			4	4		
3	C	4	Total	Cu	0	0
			4	4		
3	D	4	Total	Cu	0	0
			4	4		

- Molecule 4 is TETRAHYDROPYRAN (three-letter code: PYE) (formula: C<sub>5</sub>H<sub>10</sub>O).



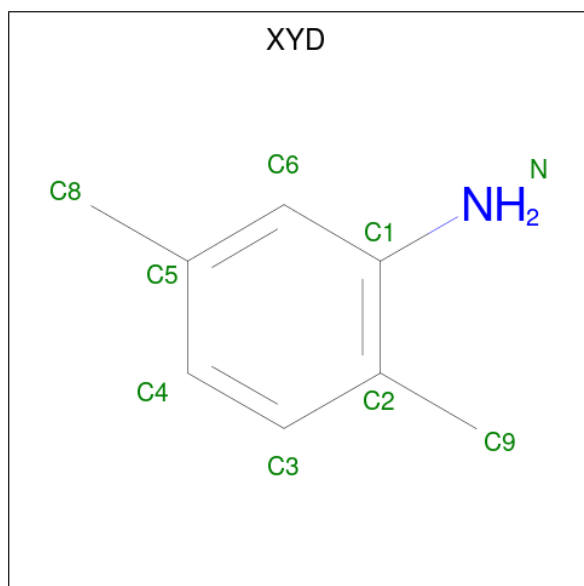
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	5	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 5 1	0	0
4	B	1	Total C O 6 5 1	0	0
4	B	1	Total C O 6 5 1	0	0
4	B	1	Total C O 6 5 1	0	0
4	B	1	Total C O 6 5 1	0	0
4	D	1	Total C O 6 5 1	0	0
4	D	1	Total C O 6 5 1	0	0
4	D	1	Total C O 6 5 1	0	0

- Molecule 5 is 2,5-DIMETHYLANILINE (three-letter code: XYD) (formula: C<sub>8</sub>H<sub>11</sub>N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 9 8 1	0	0
5	B	1	Total C N 9 8 1	0	0
5	C	1	Total C N 9 8 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	N	0	0
			9	8	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	184	Total	O	0	0
			184	184		
6	B	209	Total	O	0	0
			209	209		
6	C	199	Total	O	0	0
			199	199		
6	D	198	Total	O	0	0
			198	198		

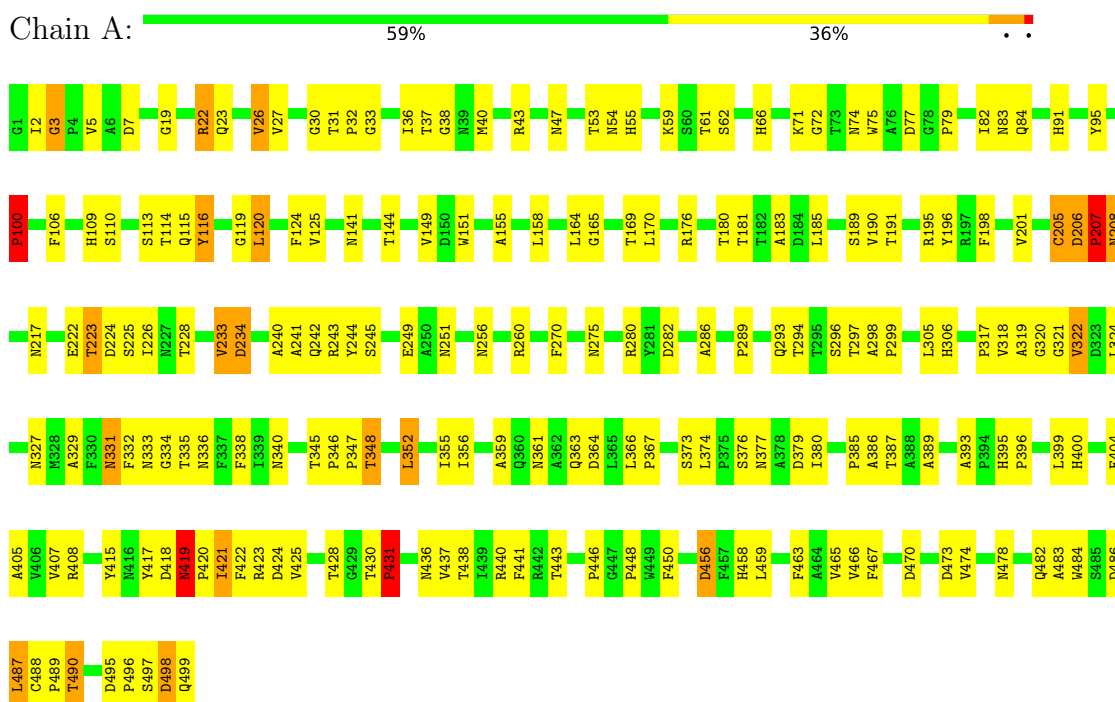


### 3 Residue-property plots

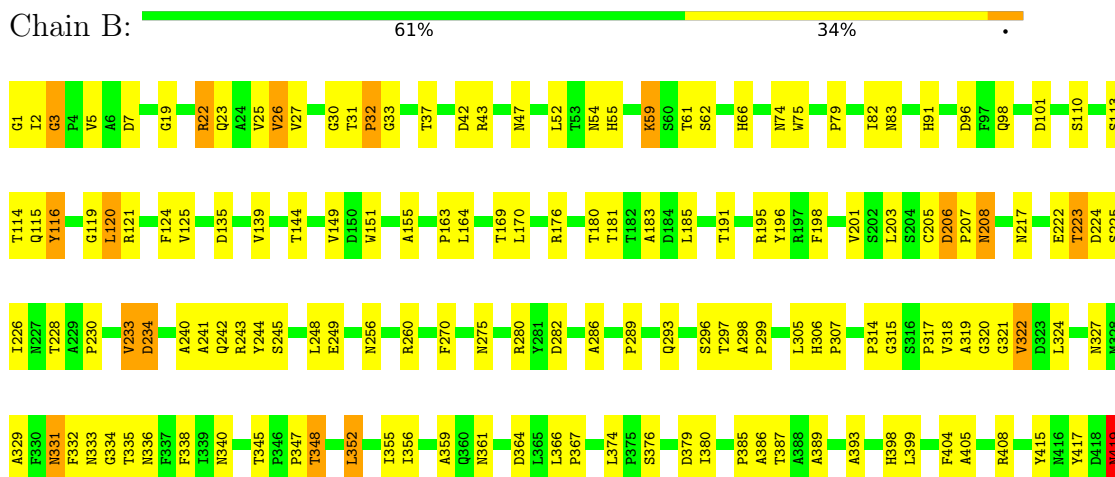
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

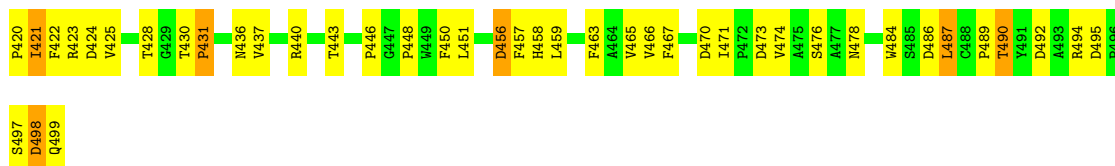
Note EDS was not executed.

- Molecule 1: LACCASE

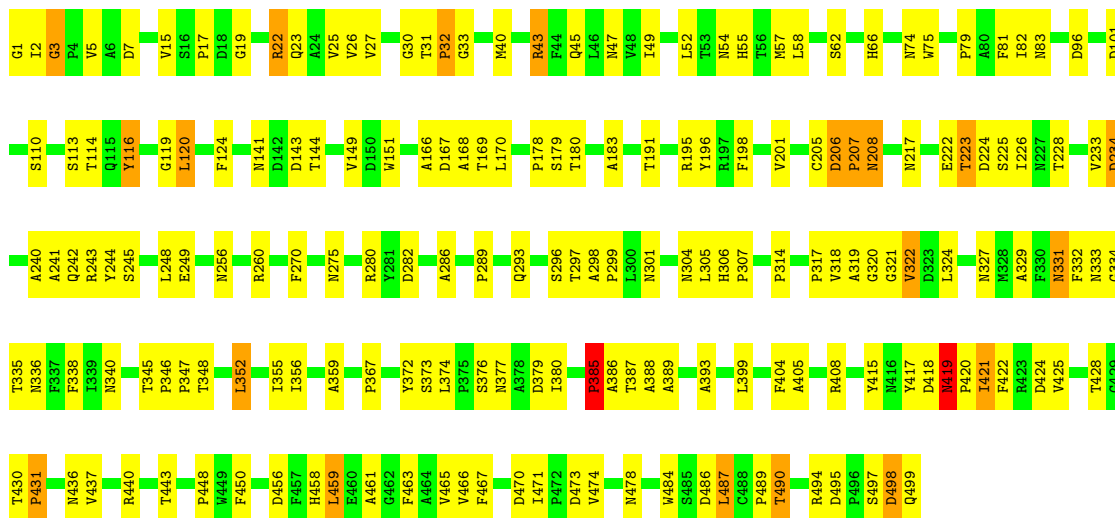


- Molecule 1: LACCASE

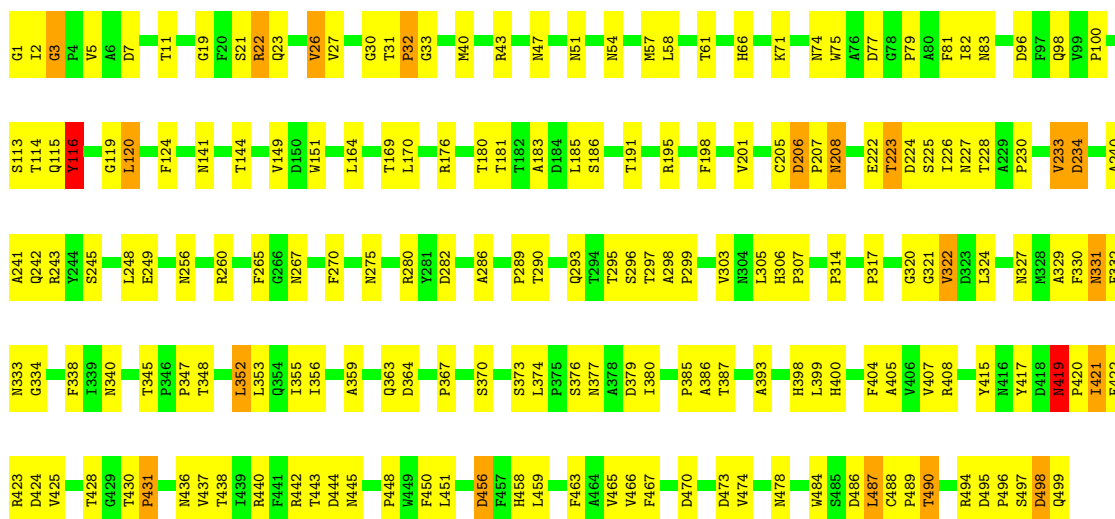




• Molecule 1: LACCASE



• Molecule 1: LACCASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.72Å 110.52Å 123.20Å 90.00° 103.44° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40	Depositor
% Data completeness (in resolution range)	93.5 (35.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.253 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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: PYE, XYD, NAG, CU

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	0.48	2/3867 (0.1%)	0.73	5/5320 (0.1%)
1	B	0.46	1/3867 (0.0%)	0.70	2/5320 (0.0%)
1	C	0.47	0/3867	0.70	4/5320 (0.1%)
1	D	0.47	0/3867	0.71	3/5320 (0.1%)
All	All	0.47	3/15468 (0.0%)	0.71	14/21280 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	PRO	N-CA	5.74	1.57	1.47
1	A	100	PRO	N-CA	5.54	1.56	1.47
1	B	431	PRO	N-CA	5.01	1.55	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	PRO	CA-N-CD	-8.80	99.18	111.50
1	A	100	PRO	CA-N-CD	-8.21	100.01	111.50
1	A	431	PRO	CA-N-CD	-7.40	101.14	111.50
1	A	100	PRO	N-CA-C	6.91	130.07	112.10
1	C	207	PRO	CA-N-CD	-6.53	102.36	111.50
1	C	431	PRO	CA-N-CD	-6.21	102.81	111.50
1	D	431	PRO	CA-N-CD	-6.13	102.91	111.50
1	B	431	PRO	CA-N-CD	-6.07	103.00	111.50
1	D	431	PRO	N-CA-C	5.77	127.11	112.10
1	B	431	PRO	N-CA-C	5.66	126.81	112.10
1	A	431	PRO	N-CA-C	5.52	126.45	112.10
1	C	431	PRO	N-CA-C	5.51	126.43	112.10
1	C	385	PRO	CA-N-CD	-5.42	103.91	111.50
1	D	116	TYR	CA-CB-CG	5.05	122.99	113.40

There are no chirality outliers.

There are no planarity outliers.

## 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	3753	0	3541	252	0
1	B	3753	0	3541	226	0
1	C	3753	0	3539	222	0
1	D	3753	0	3541	211	0
2	A	98	0	91	32	0
2	B	98	0	91	26	0
2	C	98	0	91	21	0
2	D	84	0	78	20	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	12	0	20	4	0
4	B	24	0	40	14	0
4	D	18	0	30	10	0
5	A	9	0	11	4	0
5	B	9	0	11	3	0
5	C	9	0	11	2	0
5	D	9	0	11	3	0
6	A	184	0	0	78	3
6	B	209	0	0	63	1
6	C	199	0	0	63	1
6	D	198	0	0	46	0
All	All	16286	0	14647	964	3

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 32.

All (964) 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:D:332:PHE:CZ	1:D:334:GLY:O	1.72	1.39
1:D:54:ASN:HD21	2:D:806:NAG:C1	1.44	1.30
1:B:366:LEU:HG	6:B:1525:HOH:O	1.23	1.27
1:C:436:ASN:HD21	2:C:707:NAG:C1	1.46	1.26
1:C:54:ASN:HD21	2:C:706:NAG:C1	1.48	1.26
1:A:294:THR:HB	6:A:1720:HOH:O	1.35	1.24
1:B:473:ASP:OD2	6:B:1477:HOH:O	1.58	1.19
1:A:473:ASP:OD2	6:A:1655:HOH:O	1.61	1.18
1:A:54:ASN:HD21	2:A:506:NAG:C1	1.55	1.18
1:A:436:ASN:HD21	2:A:512:NAG:C1	1.58	1.17
1:B:206:ASP:HB3	1:B:207:PRO:CD	1.77	1.15
1:D:5:VAL:HG22	6:D:1773:HOH:O	1.49	1.13
1:D:364:ASP:OD1	6:D:1717:HOH:O	1.66	1.12
1:D:436:ASN:HD21	2:D:807:NAG:C1	1.63	1.12
1:D:31:THR:HG22	1:D:32:PRO:HD3	1.31	1.12
1:A:386:ALA:HB1	1:A:431:PRO:HD3	1.12	1.09
1:B:446:PRO:HD2	6:B:1671:HOH:O	1.51	1.09
1:D:494:ARG:NH1	6:D:1516:HOH:O	1.82	1.09
1:D:498:ASP:OD1	6:D:1479:HOH:O	1.70	1.09
1:C:1:GLY:N	6:C:1468:HOH:O	1.85	1.08
1:C:336:ASN:OD1	6:C:1555:HOH:O	1.68	1.08
1:D:473:ASP:HB3	6:D:1538:HOH:O	1.53	1.07
1:C:31:THR:HG22	1:C:32:PRO:HD3	1.27	1.07
1:C:96:ASP:OD2	6:C:1522:HOH:O	1.73	1.07
1:D:386:ALA:CB	1:D:431:PRO:HD3	1.85	1.06
1:B:149:VAL:HG22	6:B:1157:HOH:O	1.55	1.06
1:B:54:ASN:HD21	2:B:606:NAG:C1	1.67	1.06
2:C:711:NAG:H61	6:C:1744:HOH:O	1.56	1.06
1:A:473:ASP:OD2	6:A:1490:HOH:O	1.71	1.05
1:C:318:VAL:HG12	6:C:1539:HOH:O	1.57	1.05
1:B:386:ALA:CB	1:B:431:PRO:HD3	1.86	1.04
1:C:22:ARG:HB2	2:C:705:NAG:H81	1.38	1.04
1:A:36:ILE:HG23	6:A:1590:HOH:O	1.55	1.04
1:D:54:ASN:ND2	2:D:806:NAG:C1	2.21	1.03
1:C:386:ALA:HB1	1:C:431:PRO:HD3	1.07	1.02
1:A:319:ALA:HB1	6:A:1515:HOH:O	1.59	1.02
2:D:805:NAG:O4	4:D:808:PYE:H22	1.58	1.01
1:B:476:SER:OG	6:B:1637:HOH:O	1.79	1.01
1:D:473:ASP:OD2	6:D:1478:HOH:O	1.79	1.01
1:C:386:ALA:CB	1:C:431:PRO:HD3	1.91	1.00
1:B:206:ASP:HB3	1:B:207:PRO:HD3	1.43	1.00
1:B:386:ALA:HB1	1:B:431:PRO:CD	1.93	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ALA:N	6:A:1530:HOH:O	1.93	0.99
1:A:31:THR:CG2	6:A:1494:HOH:O	2.09	0.98
1:C:179:SER:HB3	6:C:1534:HOH:O	1.62	0.98
1:C:436:ASN:ND2	2:C:707:NAG:C1	2.24	0.98
1:B:361:ASN:ND2	6:B:1519:HOH:O	1.90	0.98
1:C:54:ASN:ND2	2:C:706:NAG:C1	2.26	0.98
1:A:195:ARG:HG2	1:A:249:GLU:HG2	1.44	0.98
1:D:31:THR:N	6:D:1487:HOH:O	1.95	0.98
1:A:386:ALA:CB	1:A:431:PRO:HD3	1.94	0.98
1:A:498:ASP:CG	6:A:1501:HOH:O	2.03	0.97
1:D:386:ALA:HB1	1:D:431:PRO:CD	1.93	0.97
1:D:386:ALA:HB1	1:D:431:PRO:HD3	0.99	0.97
1:A:54:ASN:ND2	2:A:506:NAG:C1	2.28	0.97
1:B:364:ASP:OD2	6:B:1529:HOH:O	1.81	0.96
1:C:195:ARG:HG2	1:C:249:GLU:HG2	1.46	0.96
1:B:436:ASN:HD21	2:B:607:NAG:C1	1.78	0.96
1:C:7:ASP:HB3	6:C:1544:HOH:O	1.65	0.96
1:A:498:ASP:HA	6:A:1497:HOH:O	1.63	0.96
1:B:195:ARG:HG2	1:B:249:GLU:HG2	1.44	0.96
1:C:166:ALA:O	6:C:1508:HOH:O	1.84	0.96
1:B:473:ASP:HA	6:B:1696:HOH:O	1.66	0.96
1:A:498:ASP:OD1	6:A:1501:HOH:O	1.83	0.95
1:A:165:GLY:HA3	6:A:1650:HOH:O	1.65	0.95
1:B:386:ALA:HB1	1:B:431:PRO:HD3	0.97	0.95
1:D:195:ARG:HG2	1:D:249:GLU:HG2	1.47	0.95
1:A:31:THR:HG22	1:A:32:PRO:HD3	1.47	0.95
1:B:43:ARG:CD	6:B:1611:HOH:O	2.12	0.95
1:C:498:ASP:OD2	6:C:1495:HOH:O	1.83	0.95
1:A:364:ASP:N	6:A:1581:HOH:O	1.94	0.95
1:A:31:THR:HG22	6:A:1494:HOH:O	1.67	0.94
1:A:495:ASP:O	6:A:1425:HOH:O	1.84	0.94
1:A:361:ASN:ND2	6:A:1581:HOH:O	2.00	0.94
1:C:31:THR:CG2	1:C:32:PRO:HD3	1.98	0.94
1:C:31:THR:HB	1:C:32:PRO:HD2	1.49	0.94
1:B:473:ASP:OD2	6:B:1562:HOH:O	1.86	0.93
1:A:189:SER:HB3	6:A:1177:HOH:O	1.68	0.93
1:A:217:ASN:HD21	2:A:513:NAG:C1	1.80	0.93
1:D:332:PHE:HZ	1:D:334:GLY:O	1.42	0.93
1:B:387:THR:HG22	1:B:389:ALA:H	1.32	0.93
1:B:1:GLY:N	6:B:1496:HOH:O	2.01	0.92
1:A:164:LEU:O	6:A:1650:HOH:O	1.88	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:THR:HG23	6:C:1258:HOH:O	1.68	0.92
1:C:498:ASP:CB	6:C:1495:HOH:O	2.17	0.91
1:D:31:THR:CG2	1:D:32:PRO:HD3	1.99	0.91
2:D:807:NAG:O4	6:D:1523:HOH:O	1.85	0.91
1:C:217:ASN:HD21	2:C:711:NAG:HN2	1.17	0.91
1:B:206:ASP:HB3	1:B:207:PRO:HD2	1.54	0.90
1:C:318:VAL:HA	6:C:1465:HOH:O	1.71	0.90
1:C:458:HIS:HE2	5:C:712:XYD:H6	1.37	0.90
1:B:348:THR:OG1	6:B:1514:HOH:O	1.89	0.90
1:B:498:ASP:OD1	6:B:1474:HOH:O	1.88	0.90
1:C:473:ASP:OD2	6:C:1469:HOH:O	1.83	0.90
1:C:17:PRO:O	6:C:1509:HOH:O	1.89	0.89
1:D:293:GLN:OE1	6:D:1763:HOH:O	1.88	0.89
1:D:21:SER:O	6:D:1779:HOH:O	1.89	0.89
1:B:43:ARG:NE	6:B:1611:HOH:O	2.06	0.88
1:B:43:ARG:NH2	1:B:96:ASP:OD2	2.05	0.88
1:A:458:HIS:HE2	5:A:514:XYD:H2N	1.16	0.88
1:A:393:ALA:HB2	6:A:1435:HOH:O	1.74	0.88
1:B:42:ASP:OD1	6:B:1592:HOH:O	1.89	0.88
1:B:319:ALA:N	6:B:1614:HOH:O	1.91	0.88
1:A:387:THR:HG22	1:A:389:ALA:H	1.39	0.87
1:C:319:ALA:N	6:C:1439:HOH:O	2.03	0.87
1:C:31:THR:HG22	1:C:32:PRO:CD	2.04	0.87
1:C:101:ASP:O	6:C:1704:HOH:O	1.92	0.87
1:B:23:GLN:HB2	2:B:606:NAG:H61	1.57	0.86
1:C:386:ALA:HB1	1:C:431:PRO:CD	2.01	0.86
1:C:55:HIS:NE2	6:C:1568:HOH:O	2.08	0.86
1:A:436:ASN:ND2	2:A:512:NAG:C1	2.38	0.86
1:D:444:ASP:OD2	6:D:1764:HOH:O	1.94	0.86
4:B:608:PYE:H31	4:B:615:PYE:H12	1.58	0.85
2:A:505:NAG:C1	2:A:506:NAG:O4	2.24	0.85
1:C:1:GLY:O	6:C:1726:HOH:O	1.94	0.85
1:D:363:GLN:CB	6:D:1512:HOH:O	2.24	0.85
1:B:318:VAL:HG12	6:B:1614:HOH:O	1.77	0.85
1:D:51:ASN:O	6:D:1520:HOH:O	1.95	0.85
1:B:43:ARG:HD2	6:B:1611:HOH:O	1.76	0.85
1:D:31:THR:HB	1:D:32:PRO:HD2	1.58	0.84
1:C:143:ASP:OD1	6:C:1780:HOH:O	1.96	0.84
1:C:306:HIS:HD2	1:C:419:ASN:O	1.59	0.83
1:B:54:ASN:ND2	2:B:606:NAG:C1	2.42	0.83
1:C:55:HIS:CD2	6:C:1568:HOH:O	2.31	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:HIS:HD2	1:A:419:ASN:O	1.61	0.83
1:D:31:THR:HG22	1:D:32:PRO:CD	2.09	0.82
1:A:5:VAL:HG22	6:A:1348:HOH:O	1.78	0.82
1:A:418:ASP:O	6:A:1549:HOH:O	1.97	0.82
1:D:306:HIS:HD2	1:D:419:ASN:O	1.62	0.81
1:D:444:ASP:OD1	6:D:1472:HOH:O	1.98	0.81
4:A:508:PYE:H51	4:A:509:PYE:H11	1.62	0.81
1:C:318:VAL:CG1	6:C:1539:HOH:O	2.20	0.81
1:B:206:ASP:CB	1:B:207:PRO:CD	2.53	0.81
1:D:332:PHE:CE2	1:D:334:GLY:O	2.32	0.81
1:A:37:THR:CB	6:A:1789:HOH:O	2.28	0.80
1:B:318:VAL:CG1	6:B:1614:HOH:O	2.29	0.80
1:B:492:ASP:O	6:B:1702:HOH:O	2.00	0.80
1:B:494:ARG:NH1	6:B:1770:HOH:O	2.14	0.80
1:C:498:ASP:HB2	6:C:1495:HOH:O	1.81	0.80
4:B:608:PYE:H42	4:B:614:PYE:H51	1.64	0.80
1:A:31:THR:CG2	1:A:32:PRO:HD3	2.11	0.79
1:C:31:THR:CB	1:C:32:PRO:CD	2.61	0.79
1:D:164:LEU:HB3	6:D:1318:HOH:O	1.81	0.79
1:A:165:GLY:CA	6:A:1650:HOH:O	2.25	0.79
1:B:306:HIS:HD2	1:B:419:ASN:O	1.65	0.79
1:C:19:GLY:HA3	1:C:180:THR:HG21	1.64	0.79
1:D:473:ASP:OD2	6:D:1561:HOH:O	2.00	0.79
1:A:36:ILE:HA	6:A:1060:HOH:O	1.84	0.78
1:C:494:ARG:NH2	6:C:1547:HOH:O	2.16	0.78
1:C:31:THR:HB	1:C:32:PRO:CD	2.13	0.78
1:D:19:GLY:HA3	1:D:180:THR:HG21	1.65	0.78
1:A:355:ILE:HA	1:A:359:ALA:HB3	1.66	0.78
1:A:482:GLN:C	6:A:1530:HOH:O	2.18	0.77
2:C:705:NAG:C1	2:C:706:NAG:O4	2.32	0.77
1:D:31:THR:HB	1:D:32:PRO:CD	2.14	0.77
1:D:206:ASP:HB3	1:D:207:PRO:CD	2.15	0.77
1:A:31:THR:HB	1:A:32:PRO:HD2	1.65	0.77
1:B:19:GLY:HA3	1:B:180:THR:HG21	1.65	0.77
1:C:495:ASP:HB2	6:C:1495:HOH:O	1.85	0.77
1:B:55:HIS:NE2	6:B:1593:HOH:O	2.08	0.76
1:B:486:ASP:O	1:B:490:THR:HG22	1.85	0.76
1:B:31:THR:HB	1:B:32:PRO:HD2	1.67	0.76
1:B:473:ASP:CB	6:B:1696:HOH:O	2.34	0.76
1:D:201:VAL:HG13	1:D:243:ARG:HG3	1.65	0.76
1:C:355:ILE:HA	1:C:359:ALA:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:THR:HB	1:B:32:PRO:CD	2.15	0.76
1:D:290:THR:HG23	6:D:1524:HOH:O	1.84	0.76
1:D:355:ILE:HA	1:D:359:ALA:HB3	1.67	0.76
1:A:386:ALA:HB1	1:A:431:PRO:CD	2.05	0.76
1:A:486:ASP:O	1:A:490:THR:HG22	1.85	0.76
1:D:191:THR:HG21	6:D:1352:HOH:O	1.86	0.76
1:B:31:THR:HG22	1:B:32:PRO:HD3	1.66	0.76
1:B:355:ILE:HA	1:B:359:ALA:HB3	1.67	0.76
1:D:206:ASP:HB3	1:D:207:PRO:HD3	1.67	0.76
1:A:26:VAL:HG22	1:A:30:GLY:C	2.07	0.75
1:A:31:THR:HB	1:A:32:PRO:CD	2.16	0.75
2:B:607:NAG:H61	6:B:1721:HOH:O	1.86	0.75
1:C:387:THR:HG22	1:C:389:ALA:H	1.50	0.75
1:A:55:HIS:NE2	6:A:1572:HOH:O	2.18	0.75
1:D:26:VAL:HG22	1:D:30:GLY:C	2.06	0.75
1:B:203:LEU:HB2	6:B:1157:HOH:O	1.85	0.75
1:B:458:HIS:HE2	5:B:612:XYD:H6	1.50	0.75
4:D:808:PYE:H51	4:D:809:PYE:H12	1.67	0.75
1:A:417:TYR:O	6:A:1431:HOH:O	2.03	0.75
1:D:486:ASP:O	1:D:490:THR:HG22	1.87	0.74
1:D:31:THR:CB	1:D:32:PRO:CD	2.65	0.74
1:B:206:ASP:CB	1:B:207:PRO:HD3	2.15	0.74
1:C:49:ILE:CD1	6:C:1544:HOH:O	2.35	0.74
1:D:1:GLY:N	6:D:1471:HOH:O	1.72	0.74
1:C:31:THR:CG2	6:C:1489:HOH:O	2.36	0.74
1:C:486:ASP:O	1:C:490:THR:HG22	1.87	0.74
1:A:19:GLY:HA3	1:A:180:THR:HG21	1.68	0.74
1:D:498:ASP:CG	6:D:1737:HOH:O	2.26	0.74
1:C:332:PHE:CZ	1:C:334:GLY:O	2.41	0.73
1:A:55:HIS:CD2	6:A:1572:HOH:O	2.41	0.73
1:A:436:ASN:HD21	2:A:512:NAG:C2	2.00	0.73
1:A:446:PRO:HD2	6:A:1081:HOH:O	1.87	0.73
1:C:26:VAL:HG22	1:C:30:GLY:C	2.08	0.73
1:D:290:THR:CG2	6:D:1524:HOH:O	2.36	0.73
1:C:217:ASN:ND2	2:C:711:NAG:HN2	1.85	0.73
4:B:608:PYE:C4	4:B:614:PYE:H51	2.18	0.73
1:C:495:ASP:OD2	6:C:1677:HOH:O	2.06	0.73
1:A:201:VAL:HG13	1:A:243:ARG:HG3	1.69	0.73
1:B:26:VAL:HG22	1:B:30:GLY:C	2.08	0.73
1:B:54:ASN:HD21	2:B:606:NAG:C2	2.02	0.72
1:C:31:THR:CG2	1:C:32:PRO:CD	2.63	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:VAL:HG13	1:C:243:ARG:HG3	1.69	0.72
1:A:37:THR:HB	6:A:1789:HOH:O	1.86	0.72
1:C:372:TYR:OH	6:C:1654:HOH:O	2.08	0.72
1:A:206:ASP:HB3	1:A:207:PRO:CD	2.19	0.72
1:C:470:ASP:OD2	6:C:1469:HOH:O	2.07	0.72
1:A:164:LEU:C	6:A:1650:HOH:O	2.26	0.72
1:C:43:ARG:NH2	6:C:1522:HOH:O	2.22	0.72
1:C:143:ASP:CG	6:C:1780:HOH:O	2.27	0.72
1:D:436:ASN:ND2	2:D:807:NAG:C1	2.48	0.71
1:C:43:ARG:HE	1:C:45:GLN:CD	1.93	0.71
1:A:385:PRO:CG	2:A:512:NAG:HN2	2.03	0.71
1:B:91:HIS:CE1	6:B:1697:HOH:O	2.43	0.71
1:A:318:VAL:HA	6:A:1126:HOH:O	1.89	0.71
1:B:201:VAL:HG13	1:B:243:ARG:HG3	1.70	0.71
1:B:217:ASN:OD1	2:B:611:NAG:C1	2.37	0.71
1:A:37:THR:OG1	6:A:1789:HOH:O	2.08	0.71
1:C:498:ASP:CG	6:C:1495:HOH:O	2.22	0.70
2:A:505:NAG:C1	2:A:506:NAG:HO4	2.05	0.70
1:B:366:LEU:CG	6:B:1525:HOH:O	2.00	0.70
1:C:385:PRO:HD3	1:C:436:ASN:OD1	1.92	0.70
1:B:31:THR:HG23	1:B:119:GLY:HA2	1.73	0.70
1:C:31:THR:HG22	6:C:1489:HOH:O	1.91	0.70
1:A:72:GLY:N	6:A:1223:HOH:O	2.13	0.70
1:B:385:PRO:HD3	1:B:436:ASN:OD1	1.91	0.69
1:C:40:MET:CE	6:C:1007:HOH:O	2.40	0.69
1:C:7:ASP:OD1	1:D:295:THR:OG1	2.11	0.69
1:A:31:THR:CB	1:A:32:PRO:CD	2.70	0.69
1:A:327:ASN:HD21	1:A:385:PRO:HG2	1.58	0.69
1:C:49:ILE:HG13	6:C:1544:HOH:O	1.92	0.69
1:C:74:ASN:H	1:C:478:ASN:ND2	1.91	0.69
1:D:31:THR:HG23	1:D:119:GLY:HA2	1.73	0.69
1:D:74:ASN:H	1:D:478:ASN:ND2	1.91	0.69
1:D:417:TYR:OH	6:D:1461:HOH:O	2.08	0.69
1:D:31:THR:CG2	1:D:32:PRO:CD	2.69	0.69
1:B:473:ASP:OD1	6:B:1696:HOH:O	2.09	0.69
1:A:31:THR:HG23	1:A:119:GLY:HA2	1.75	0.68
1:D:74:ASN:HD22	1:D:352:LEU:HG	1.58	0.68
1:B:332:PHE:CZ	1:B:334:GLY:O	2.46	0.68
1:C:458:HIS:HE2	5:C:712:XYD:C6	2.05	0.68
1:D:293:GLN:HB3	6:D:1452:HOH:O	1.93	0.68
1:A:363:GLN:CB	6:A:1581:HOH:O	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASN:H	1:B:478:ASN:ND2	1.91	0.68
1:C:31:THR:HG23	1:C:119:GLY:HA2	1.74	0.68
1:D:458:HIS:HE2	5:D:814:XYD:H6	1.59	0.68
1:A:206:ASP:HB3	1:A:207:PRO:HD2	1.76	0.67
1:C:31:THR:O	1:C:33:GLY:N	2.27	0.67
1:C:234:ASP:OD2	1:C:296:SER:HA	1.94	0.67
1:D:234:ASP:OD2	1:D:296:SER:HA	1.94	0.67
1:B:31:THR:CB	1:B:32:PRO:CD	2.73	0.67
1:B:113:SER:O	6:B:1361:HOH:O	2.13	0.67
1:B:31:THR:CG2	1:B:32:PRO:HD3	2.25	0.67
1:A:2:ILE:O	6:A:1060:HOH:O	2.12	0.66
1:B:366:LEU:CD2	6:B:1525:HOH:O	2.37	0.66
1:B:379:ASP:OD2	6:B:1444:HOH:O	2.14	0.66
1:C:327:ASN:HD21	1:C:385:PRO:HG2	1.59	0.66
1:B:499:GLN:O	6:B:1429:HOH:O	2.11	0.66
1:C:74:ASN:HD22	1:C:352:LEU:HG	1.61	0.66
1:C:317:PRO:O	6:C:1465:HOH:O	2.12	0.66
1:A:363:GLN:CA	6:A:1581:HOH:O	2.43	0.66
1:D:31:THR:O	1:D:33:GLY:N	2.27	0.66
1:B:320:GLY:O	1:B:322:VAL:N	2.28	0.66
1:A:31:THR:HG22	1:A:32:PRO:CD	2.24	0.66
1:C:470:ASP:OD2	1:C:473:ASP:OD2	2.13	0.66
1:A:234:ASP:OD2	1:A:296:SER:HA	1.95	0.65
1:B:458:HIS:HE2	5:B:612:XYD:C6	2.09	0.65
1:B:234:ASP:OD2	1:B:296:SER:HA	1.95	0.65
4:D:808:PYE:H11	4:D:810:PYE:H11	1.77	0.65
1:A:31:THR:O	1:A:33:GLY:N	2.29	0.65
1:A:2:ILE:O	6:A:1590:HOH:O	2.13	0.65
1:A:74:ASN:H	1:A:478:ASN:ND2	1.94	0.65
1:A:473:ASP:CG	6:A:1490:HOH:O	2.25	0.65
1:B:470:ASP:OD2	1:B:473:ASP:OD2	2.15	0.65
1:C:497:SER:C	1:C:499:GLN:H	2.01	0.64
4:A:508:PYE:H51	4:A:509:PYE:C1	2.27	0.64
1:B:327:ASN:HD21	1:B:385:PRO:HG2	1.61	0.64
1:B:486:ASP:O	1:B:489:PRO:HD2	1.97	0.64
1:A:54:ASN:HD21	2:A:506:NAG:C2	2.10	0.64
1:B:366:LEU:HD13	6:B:1733:HOH:O	1.96	0.64
1:D:497:SER:C	1:D:499:GLN:H	2.01	0.64
1:C:499:GLN:HB3	6:C:1008:HOH:O	1.97	0.64
2:D:805:NAG:C1	2:D:806:NAG:O4	2.46	0.64
1:C:320:GLY:O	1:C:322:VAL:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:ND2	1:A:83:ASN:HD22	1.96	0.63
1:C:222:GLU:HB3	1:C:245:SER:HB2	1.80	0.63
1:A:497:SER:C	1:A:499:GLN:H	2.02	0.63
1:B:74:ASN:ND2	1:B:83:ASN:HD22	1.96	0.63
1:D:74:ASN:ND2	1:D:83:ASN:HD22	1.96	0.63
1:A:114:THR:HA	1:A:456:ASP:OD1	1.99	0.63
1:A:385:PRO:HD3	1:A:436:ASN:OD1	1.97	0.63
1:B:74:ASN:HD22	1:B:352:LEU:HG	1.62	0.63
1:A:320:GLY:O	1:A:322:VAL:N	2.32	0.63
1:A:333:ASN:ND2	2:A:510:NAG:C1	2.62	0.63
1:B:348:THR:CG2	6:B:1514:HOH:O	2.46	0.63
1:B:428:THR:HA	1:B:437:VAL:HG21	1.80	0.63
2:C:705:NAG:C1	2:C:706:NAG:HO4	2.12	0.63
1:D:1:GLY:N	6:D:1575:HOH:O	2.31	0.63
1:D:222:GLU:HB3	1:D:245:SER:HB2	1.79	0.63
1:A:470:ASP:OD2	1:A:473:ASP:OD2	2.17	0.62
1:B:230:PRO:HD3	6:B:1329:HOH:O	1.99	0.62
1:B:393:ALA:HB1	1:B:430:THR:HG22	1.80	0.62
1:A:74:ASN:HD22	1:A:352:LEU:HG	1.64	0.62
1:B:495:ASP:N	6:B:1238:HOH:O	2.31	0.62
1:B:497:SER:C	1:B:499:GLN:H	2.01	0.62
1:D:470:ASP:OD2	1:D:473:ASP:OD2	2.16	0.62
1:C:114:THR:HA	1:C:456:ASP:OD1	1.98	0.62
2:C:709:NAG:H5	2:C:710:NAG:O4	2.00	0.62
1:A:222:GLU:HB3	1:A:245:SER:HB2	1.82	0.62
2:B:606:NAG:H4	4:B:616:PYE:H12	1.80	0.61
1:B:436:ASN:ND2	2:B:607:NAG:C1	2.59	0.61
1:D:100:PRO:HA	6:D:1330:HOH:O	1.99	0.61
1:A:499:GLN:N	6:A:1425:HOH:O	2.33	0.61
1:B:155:ALA:H	2:B:605:NAG:H83	1.65	0.61
1:A:385:PRO:HG3	2:A:512:NAG:HN2	1.65	0.61
1:A:329:ALA:H	1:A:340:ASN:ND2	1.98	0.61
1:D:364:ASP:CG	6:D:1717:HOH:O	2.25	0.61
1:C:486:ASP:O	1:C:489:PRO:HD2	2.01	0.61
1:A:180:THR:HG22	1:A:183:ALA:HB2	1.82	0.61
1:B:31:THR:O	1:B:33:GLY:N	2.33	0.61
1:A:428:THR:HA	1:A:437:VAL:HG21	1.83	0.61
2:B:605:NAG:O7	2:B:605:NAG:H3	1.99	0.61
1:B:471:ILE:HG13	6:B:1119:HOH:O	2.00	0.61
1:D:486:ASP:O	1:D:489:PRO:HD2	2.01	0.61
1:A:66:HIS:CE1	1:A:241:ALA:HB1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PRO:HG3	2:A:512:NAG:C1	2.30	0.60
2:A:507:NAG:C1	2:A:512:NAG:O4	2.49	0.60
1:B:121:ARG:HD2	6:B:1157:HOH:O	2.01	0.60
1:B:164:LEU:HG	6:B:1271:HOH:O	2.01	0.60
1:B:116:TYR:CE1	1:B:205:CYS:SG	2.95	0.60
1:D:393:ALA:HB1	1:D:430:THR:HG22	1.84	0.60
1:A:53:THR:OG1	6:A:1630:HOH:O	1.86	0.60
2:B:611:NAG:H4	2:B:613:NAG:C1	2.32	0.60
1:C:74:ASN:ND2	1:C:83:ASN:HD22	1.99	0.60
1:D:43:ARG:NH2	1:D:96:ASP:OD2	2.35	0.60
1:D:327:ASN:HD21	1:D:385:PRO:HG2	1.67	0.60
1:B:114:THR:HA	1:B:456:ASP:OD1	2.02	0.59
1:B:1:GLY:N	6:B:1473:HOH:O	1.73	0.59
1:C:40:MET:HE1	6:C:1007:HOH:O	2.00	0.59
1:D:320:GLY:O	1:D:322:VAL:N	2.33	0.59
1:A:486:ASP:O	1:A:489:PRO:HD2	2.02	0.59
1:C:306:HIS:CD2	1:C:419:ASN:O	2.50	0.59
1:B:98:GLN:NE2	6:B:1332:HOH:O	2.35	0.59
2:B:605:NAG:H62	4:B:608:PYE:H22	1.83	0.59
1:C:113:SER:OG	1:C:114:THR:N	2.30	0.59
2:A:505:NAG:O4	4:A:508:PYE:H21	2.02	0.59
1:D:424:ASP:OD1	1:D:425:VAL:HG23	2.01	0.59
1:C:22:ARG:HB2	2:C:705:NAG:C8	2.25	0.59
1:A:424:ASP:OD1	1:A:425:VAL:HG23	2.02	0.59
1:C:331:ASN:HD22	1:C:332:PHE:H	1.50	0.59
1:D:494:ARG:NH2	6:D:1026:HOH:O	2.34	0.59
1:B:116:TYR:HD2	6:B:1313:HOH:O	1.84	0.58
1:B:424:ASP:OD1	1:B:425:VAL:HG23	2.03	0.58
1:D:27:VAL:CG2	1:D:120:LEU:HD13	2.32	0.58
1:A:155:ALA:N	2:A:505:NAG:H81	2.18	0.58
2:A:507:NAG:O7	2:A:512:NAG:H61	2.02	0.58
1:C:167:ASP:O	6:C:1450:HOH:O	2.17	0.58
1:C:40:MET:HE2	6:C:1007:HOH:O	2.01	0.58
1:D:114:THR:HA	1:D:456:ASP:OD1	2.03	0.58
2:D:811:NAG:C1	2:D:812:NAG:O4	2.51	0.58
1:C:49:ILE:HD12	6:C:1544:HOH:O	1.99	0.58
1:B:66:HIS:CE1	1:B:241:ALA:HB1	2.39	0.58
1:D:473:ASP:CB	6:D:1538:HOH:O	2.29	0.58
1:D:332:PHE:CZ	1:D:334:GLY:C	2.71	0.58
1:C:498:ASP:N	6:C:1495:HOH:O	2.19	0.58
1:D:331:ASN:HD22	1:D:332:PHE:H	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLU:HB3	1:B:245:SER:HB2	1.86	0.58
1:C:74:ASN:H	1:C:478:ASN:HD22	1.50	0.58
1:D:32:PRO:N	6:D:1487:HOH:O	2.36	0.58
1:C:66:HIS:CE1	1:C:241:ALA:HB1	2.38	0.57
1:D:428:THR:HA	1:D:437:VAL:HG21	1.84	0.57
1:A:385:PRO:HG3	1:A:436:ASN:OD1	2.04	0.57
1:A:91:HIS:CE1	6:A:1571:HOH:O	2.56	0.57
1:A:224:ASP:O	1:A:225:SER:HB2	2.04	0.57
1:A:331:ASN:HD22	1:A:332:PHE:H	1.50	0.57
1:C:180:THR:HG22	1:C:183:ALA:HB2	1.85	0.57
1:D:74:ASN:H	1:D:478:ASN:HD22	1.52	0.57
1:D:334:GLY:C	6:D:1141:HOH:O	2.42	0.57
1:A:71:LYS:HD2	6:A:1176:HOH:O	2.04	0.57
1:B:74:ASN:H	1:B:478:ASN:HD22	1.50	0.57
1:B:473:ASP:CA	6:B:1696:HOH:O	2.30	0.57
1:B:473:ASP:CG	6:B:1696:HOH:O	2.43	0.57
1:C:333:ASN:ND2	1:C:338:PHE:CE2	2.72	0.57
1:D:22:ARG:HD3	1:D:23:GLN:O	2.05	0.57
1:B:489:PRO:HD3	6:B:1383:HOH:O	2.03	0.57
1:D:333:ASN:ND2	1:D:338:PHE:CE2	2.73	0.57
1:A:484:TRP:HA	1:A:487:LEU:HD22	1.87	0.56
1:C:424:ASP:OD1	1:C:425:VAL:HG23	2.04	0.56
1:A:361:ASN:CG	6:A:1581:HOH:O	2.36	0.56
1:A:31:THR:HG23	1:A:119:GLY:CA	2.35	0.56
1:A:380:ILE:HD11	1:A:443:THR:HG23	1.88	0.56
1:B:180:THR:HG22	1:B:183:ALA:HB2	1.85	0.56
1:B:446:PRO:CD	6:B:1671:HOH:O	2.26	0.56
1:A:2:ILE:O	1:A:3:GLY:O	2.24	0.56
4:B:616:PYE:H11	6:B:1018:HOH:O	2.05	0.56
1:C:208:ASN:C	1:C:208:ASN:HD22	2.08	0.56
1:A:333:ASN:HD21	2:A:510:NAG:H5	1.71	0.56
1:D:180:THR:HG22	1:D:183:ALA:HB2	1.87	0.56
1:C:428:THR:HA	1:C:437:VAL:HG21	1.86	0.56
1:A:31:THR:CG2	1:A:32:PRO:CD	2.81	0.56
1:B:333:ASN:ND2	1:B:338:PHE:CE2	2.74	0.56
1:A:498:ASP:HB3	6:A:1586:HOH:O	2.05	0.56
1:B:27:VAL:CG2	1:B:120:LEU:HD13	2.35	0.55
1:C:27:VAL:CG2	1:C:120:LEU:HD13	2.37	0.55
1:D:458:HIS:HE2	5:D:814:XYD:C6	2.18	0.55
1:A:363:GLN:N	6:A:1581:HOH:O	2.39	0.55
1:C:498:ASP:CG	6:C:1394:HOH:O	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLY:N	6:A:1789:HOH:O	2.38	0.55
1:B:116:TYR:HB3	6:B:1313:HOH:O	2.06	0.55
1:C:335:THR:OG1	1:C:336:ASN:ND2	2.39	0.55
1:D:267:ASN:HB2	6:D:1129:HOH:O	2.07	0.55
4:D:808:PYE:H51	4:D:809:PYE:C1	2.35	0.55
4:B:608:PYE:C3	4:B:615:PYE:H12	2.33	0.55
1:D:353:LEU:HD11	6:D:1669:HOH:O	2.06	0.55
1:D:54:ASN:HD21	2:D:806:NAG:C2	2.17	0.55
1:D:66:HIS:CE1	1:D:241:ALA:HB1	2.41	0.55
1:A:436:ASN:ND2	2:A:512:NAG:C2	2.68	0.55
1:C:380:ILE:HD11	1:C:443:THR:HG23	1.88	0.55
1:B:340:ASN:ND2	6:B:1548:HOH:O	2.40	0.55
1:B:484:TRP:HA	1:B:487:LEU:HD22	1.89	0.55
1:C:347:PRO:HD3	1:C:367:PRO:HD3	1.87	0.55
4:D:808:PYE:C1	4:D:810:PYE:H11	2.35	0.55
1:A:54:ASN:CG	2:A:506:NAG:C1	2.76	0.54
1:A:298:ALA:N	1:A:299:PRO:HD3	2.22	0.54
1:C:256:ASN:HB3	1:C:289:PRO:HG3	1.89	0.54
1:C:298:ALA:N	1:C:299:PRO:HD3	2.22	0.54
1:A:217:ASN:ND2	2:A:513:NAG:C1	2.61	0.54
1:A:385:PRO:HG3	2:A:512:NAG:N2	2.22	0.54
1:D:490:THR:HG23	6:D:1025:HOH:O	2.06	0.54
1:A:404:PHE:O	1:A:422:PHE:HA	2.07	0.54
1:D:116:TYR:CE1	1:D:205:CYS:SG	3.00	0.54
1:A:446:PRO:CD	6:A:1081:HOH:O	2.49	0.54
1:C:393:ALA:HB1	1:C:430:THR:HG22	1.90	0.54
1:A:79:PRO:HB2	1:A:82:ILE:HB	1.90	0.54
1:B:31:THR:HG23	1:B:119:GLY:CA	2.36	0.54
1:C:385:PRO:HG3	2:C:707:NAG:C1	2.37	0.54
1:C:223:THR:HG23	1:C:228:THR:OG1	2.07	0.54
1:D:223:THR:HG23	1:D:228:THR:OG1	2.08	0.54
1:A:113:SER:OG	1:A:114:THR:N	2.38	0.54
1:A:260:ARG:HB3	1:A:270:PHE:CE1	2.42	0.54
1:A:347:PRO:HD3	1:A:367:PRO:HD3	1.90	0.54
1:A:499:GLN:CA	6:A:1425:HOH:O	2.54	0.54
1:D:191:THR:HG22	1:D:282:ASP:OD2	2.07	0.54
1:D:224:ASP:O	1:D:225:SER:HB2	2.08	0.54
1:B:331:ASN:HD22	1:B:332:PHE:H	1.55	0.54
1:B:385:PRO:HG3	1:B:436:ASN:OD1	2.08	0.54
1:A:40:MET:CE	6:A:1009:HOH:O	2.56	0.54
1:C:141:ASN:HB2	6:C:1106:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASN:ND2	1:D:352:LEU:HG	2.22	0.53
1:A:223:THR:HG23	1:A:228:THR:OG1	2.07	0.53
1:C:471:ILE:HG13	6:C:1440:HOH:O	2.08	0.53
1:D:442:ARG:CB	6:D:1344:HOH:O	2.55	0.53
1:A:27:VAL:CG2	1:A:120:LEU:HD13	2.38	0.53
1:B:404:PHE:O	1:B:422:PHE:HA	2.09	0.53
1:B:458:HIS:NE2	5:B:612:XYD:H6	2.19	0.53
1:B:113:SER:OG	1:B:114:THR:N	2.37	0.53
1:A:499:GLN:HB3	6:A:1006:HOH:O	2.07	0.53
1:B:27:VAL:HG22	1:B:120:LEU:HD13	1.91	0.53
1:C:260:ARG:HB3	1:C:270:PHE:CE1	2.44	0.53
1:D:484:TRP:HA	1:D:487:LEU:HD22	1.90	0.53
1:A:74:ASN:H	1:A:478:ASN:HD22	1.54	0.53
1:C:54:ASN:CG	2:C:706:NAG:C1	2.77	0.53
1:C:179:SER:CB	6:C:1534:HOH:O	2.37	0.53
1:A:333:ASN:ND2	1:A:338:PHE:CE2	2.77	0.53
1:C:327:ASN:HD22	2:C:707:NAG:H5	1.73	0.53
1:A:306:HIS:CD2	1:A:419:ASN:O	2.52	0.53
1:B:256:ASN:HB3	1:B:289:PRO:HG3	1.91	0.52
1:C:224:ASP:O	1:C:225:SER:HB2	2.09	0.52
1:C:404:PHE:O	1:C:422:PHE:HA	2.08	0.52
1:A:22:ARG:HD3	1:A:23:GLN:O	2.09	0.52
1:A:473:ASP:OD2	6:A:1484:HOH:O	2.18	0.52
1:B:387:THR:HG22	1:B:389:ALA:N	2.14	0.52
1:C:329:ALA:H	1:C:340:ASN:ND2	2.07	0.52
1:B:234:ASP:HB2	1:B:298:ALA:HB3	1.89	0.52
1:D:74:ASN:HD21	1:D:83:ASN:HD22	1.57	0.52
1:C:27:VAL:HG22	1:C:120:LEU:HD13	1.91	0.52
1:A:82:ILE:HG22	1:A:83:ASN:OD1	2.09	0.52
1:B:348:THR:HG22	6:B:1686:HOH:O	2.10	0.52
2:C:707:NAG:O4	2:C:708:NAG:C1	2.58	0.52
1:D:82:ILE:HG22	1:D:83:ASN:OD1	2.09	0.52
1:D:306:HIS:CD2	1:D:419:ASN:HB3	2.44	0.52
1:D:347:PRO:HD3	1:D:367:PRO:HD3	1.90	0.52
1:B:79:PRO:HB2	1:B:82:ILE:HB	1.92	0.52
1:B:495:ASP:HB2	1:B:498:ASP:HB2	1.91	0.52
1:C:22:ARG:HD3	1:C:23:GLN:O	2.09	0.52
1:C:484:TRP:HA	1:C:487:LEU:HD22	1.91	0.52
1:D:495:ASP:HB2	1:D:498:ASP:HB2	1.91	0.52
1:C:234:ASP:HB2	1:C:298:ALA:HB3	1.91	0.52
1:D:293:GLN:NE2	6:D:1667:HOH:O	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ASN:HB3	1:C:338:PHE:HB2	1.91	0.52
1:C:31:THR:HG23	1:C:119:GLY:CA	2.38	0.52
1:C:329:ALA:H	1:C:340:ASN:HD21	1.58	0.52
1:D:223:THR:CG2	1:D:228:THR:OG1	2.57	0.52
1:A:201:VAL:HG13	1:A:243:ARG:CG	2.39	0.51
1:B:31:THR:HG22	1:B:32:PRO:CD	2.39	0.51
1:B:306:HIS:CD2	1:B:419:ASN:HB3	2.44	0.51
2:D:805:NAG:C4	4:D:808:PYE:H22	2.38	0.51
1:C:208:ASN:C	1:C:208:ASN:ND2	2.63	0.51
1:C:380:ILE:CD1	1:C:443:THR:HG23	2.40	0.51
1:D:74:ASN:HD21	1:D:448:PRO:HG2	1.75	0.51
1:A:380:ILE:CD1	1:A:443:THR:HG23	2.40	0.51
1:B:191:THR:HG22	1:B:282:ASP:OD2	2.10	0.51
2:C:707:NAG:H61	2:C:708:NAG:O7	2.11	0.51
1:B:74:ASN:HD21	1:B:83:ASN:HD22	1.56	0.51
1:B:298:ALA:N	1:B:299:PRO:HD3	2.26	0.51
1:D:404:PHE:O	1:D:422:PHE:HA	2.09	0.51
1:A:191:THR:HG22	1:A:282:ASP:OD2	2.10	0.51
1:A:393:ALA:HB1	1:A:430:THR:HG22	1.91	0.51
1:D:333:ASN:OD1	1:D:333:ASN:O	2.28	0.51
2:B:605:NAG:O7	2:B:606:NAG:H62	2.11	0.51
1:C:54:ASN:HD21	2:C:706:NAG:C2	2.20	0.51
1:C:82:ILE:HG22	1:C:83:ASN:OD1	2.10	0.51
1:D:79:PRO:HB2	1:D:82:ILE:HB	1.92	0.51
2:D:805:NAG:O4	4:D:808:PYE:C2	2.46	0.51
1:B:191:THR:HG21	6:B:1759:HOH:O	2.09	0.51
1:B:223:THR:HG23	1:B:228:THR:OG1	2.10	0.51
1:B:352:LEU:HD13	1:B:484:TRP:CZ2	2.46	0.51
1:C:79:PRO:HB2	1:C:82:ILE:HB	1.92	0.51
1:D:176:ARG:HG3	1:D:185:LEU:HD21	1.92	0.51
1:D:458:HIS:NE2	5:D:814:XYD:H6	2.25	0.51
1:A:332:PHE:CZ	1:A:334:GLY:O	2.64	0.51
1:A:499:GLN:HA	6:A:1425:HOH:O	2.11	0.51
1:B:74:ASN:ND2	1:B:352:LEU:HG	2.25	0.51
1:B:306:HIS:CD2	1:B:419:ASN:O	2.55	0.51
1:A:348:THR:N	6:A:1511:HOH:O	1.91	0.51
1:B:234:ASP:OD2	1:B:297:THR:N	2.41	0.51
1:D:54:ASN:CG	2:D:806:NAG:C1	2.79	0.50
1:A:190:VAL:N	6:A:1177:HOH:O	2.44	0.50
1:C:322:VAL:HG22	1:C:379:ASP:O	2.11	0.50
1:D:298:ALA:N	1:D:299:PRO:HD3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASP:HB2	1:A:298:ALA:HB3	1.92	0.50
1:A:331:ASN:HB3	1:A:338:PHE:HB2	1.92	0.50
1:C:2:ILE:O	1:C:3:GLY:O	2.28	0.50
1:C:116:TYR:CE1	1:C:205:CYS:SG	3.04	0.50
1:D:256:ASN:HB3	1:D:289:PRO:HG3	1.93	0.50
1:B:322:VAL:HG22	1:B:379:ASP:HB2	1.93	0.50
1:C:380:ILE:HD11	1:C:443:THR:CG2	2.41	0.50
1:B:336:ASN:ND2	2:B:610:NAG:H5	2.25	0.50
1:C:234:ASP:OD2	1:C:297:THR:N	2.43	0.50
1:A:74:ASN:HD21	1:A:448:PRO:HG2	1.77	0.50
1:A:473:ASP:CB	6:A:1490:HOH:O	2.59	0.50
1:B:149:VAL:HB	1:B:170:LEU:HB2	1.93	0.50
1:B:347:PRO:HD3	1:B:367:PRO:HD3	1.93	0.50
4:B:616:PYE:C1	6:B:1018:HOH:O	2.58	0.50
1:D:61:THR:OG1	1:D:115:GLN:NE2	2.44	0.50
1:D:352:LEU:O	1:D:356:ILE:HG13	2.11	0.50
1:A:338:PHE:CZ	2:A:510:NAG:H62	2.47	0.50
1:A:366:LEU:HB3	6:A:1399:HOH:O	2.10	0.50
1:B:116:TYR:CD2	6:B:1313:HOH:O	2.55	0.50
1:C:418:ASP:OD1	6:C:1210:HOH:O	2.19	0.50
1:D:331:ASN:HB3	1:D:338:PHE:HB2	1.94	0.50
1:D:31:THR:HG23	1:D:119:GLY:CA	2.40	0.50
1:A:141:ASN:HB2	6:A:1543:HOH:O	2.11	0.50
1:A:319:ALA:CB	6:A:1515:HOH:O	2.37	0.50
1:C:331:ASN:ND2	1:C:332:PHE:H	2.10	0.50
1:D:306:HIS:CD2	1:D:419:ASN:O	2.53	0.50
1:A:74:ASN:ND2	1:A:448:PRO:HD2	2.26	0.49
1:A:306:HIS:CD2	1:A:419:ASN:HB3	2.46	0.49
1:A:322:VAL:HG22	1:A:379:ASP:O	2.12	0.49
1:A:380:ILE:HD11	1:A:443:THR:CG2	2.41	0.49
1:B:224:ASP:O	1:B:225:SER:HB2	2.12	0.49
1:D:208:ASN:C	1:D:208:ASN:HD22	2.15	0.49
1:D:234:ASP:HB2	1:D:298:ALA:HB3	1.93	0.49
1:A:74:ASN:HD21	1:A:83:ASN:HD22	1.57	0.49
1:B:331:ASN:HB3	1:B:338:PHE:HB2	1.93	0.49
1:D:2:ILE:O	1:D:3:GLY:O	2.30	0.49
1:A:234:ASP:OD2	1:A:297:THR:N	2.43	0.49
1:A:346:PRO:HG3	6:A:1553:HOH:O	2.12	0.49
1:D:61:THR:CB	1:D:115:GLN:HE22	2.25	0.49
1:A:40:MET:HE2	6:A:1009:HOH:O	2.11	0.49
4:B:608:PYE:C3	4:B:614:PYE:H51	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:THR:HG22	1:C:282:ASP:OD2	2.13	0.49
1:B:201:VAL:HG13	1:B:243:ARG:CG	2.42	0.49
1:C:322:VAL:HG22	1:C:379:ASP:HB2	1.94	0.49
1:D:40:MET:CE	6:D:1017:HOH:O	2.61	0.49
1:D:40:MET:HE1	6:D:1017:HOH:O	2.12	0.49
1:A:352:LEU:O	1:A:356:ILE:HG13	2.12	0.49
1:A:458:HIS:NE2	5:A:514:XYD:H6	2.27	0.49
1:D:74:ASN:ND2	1:D:448:PRO:HD2	2.27	0.49
1:A:331:ASN:ND2	1:A:332:PHE:H	2.11	0.49
2:B:605:NAG:H4	4:B:608:PYE:C2	2.41	0.49
1:C:74:ASN:ND2	1:C:448:PRO:HD2	2.28	0.49
1:C:318:VAL:HA	6:C:1439:HOH:O	2.12	0.49
1:D:260:ARG:HB3	1:D:270:PHE:CE1	2.48	0.49
1:A:329:ALA:H	1:A:340:ASN:HD21	1.61	0.49
1:C:240:ALA:O	1:C:241:ALA:HB3	2.13	0.49
1:D:240:ALA:O	1:D:241:ALA:HB3	2.13	0.49
1:D:327:ASN:HD21	1:D:385:PRO:CG	2.25	0.49
1:A:338:PHE:HZ	2:A:510:NAG:H62	1.76	0.49
1:A:169:THR:OG1	1:A:275:ASN:ND2	2.45	0.49
1:D:113:SER:OG	1:D:114:THR:N	2.45	0.49
1:B:22:ARG:HD3	1:B:23:GLN:O	2.13	0.48
1:C:74:ASN:ND2	1:C:352:LEU:HG	2.25	0.48
1:D:329:ALA:H	1:D:340:ASN:HD21	1.61	0.48
1:A:458:HIS:HE2	5:A:514:XYD:H6	1.78	0.48
1:D:201:VAL:HG13	1:D:243:ARG:CG	2.37	0.48
1:A:27:VAL:HG22	1:A:120:LEU:HD13	1.95	0.48
2:A:505:NAG:C1	2:A:506:NAG:C4	2.91	0.48
1:B:335:THR:OG1	1:B:336:ASN:ND2	2.46	0.48
1:B:380:ILE:CD1	1:B:443:THR:HG23	2.43	0.48
1:C:49:ILE:CG1	6:C:1544:HOH:O	2.49	0.48
1:A:322:VAL:HG22	1:A:379:ASP:HB2	1.96	0.48
1:A:490:THR:HG23	6:A:1037:HOH:O	2.14	0.48
1:B:55:HIS:NE2	6:B:1488:HOH:O	2.35	0.48
1:B:380:ILE:HD11	1:B:443:THR:HG23	1.96	0.48
1:C:149:VAL:HB	1:C:170:LEU:HB2	1.95	0.48
1:A:54:ASN:OD1	2:A:506:NAG:C1	2.62	0.48
1:B:314:PRO:HG2	1:B:440:ARG:HB3	1.95	0.48
4:B:608:PYE:H32	4:B:614:PYE:H51	1.95	0.48
1:C:333:ASN:C	1:C:333:ASN:OD1	2.51	0.48
1:C:497:SER:C	1:C:499:GLN:N	2.67	0.48
1:C:206:ASP:HB3	1:C:207:PRO:CD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:HIS:CD2	1:C:419:ASN:HB3	2.49	0.48
1:D:230:PRO:HD3	6:D:1146:HOH:O	2.12	0.48
1:D:322:VAL:HG22	1:D:379:ASP:HB2	1.96	0.48
1:B:240:ALA:O	1:B:241:ALA:HB3	2.14	0.48
1:B:380:ILE:O	1:B:440:ARG:HA	2.14	0.48
1:C:15:VAL:HG23	6:C:1687:HOH:O	2.12	0.48
1:C:376:SER:HB3	1:C:470:ASP:HB2	1.95	0.48
1:D:379:ASP:OD2	6:D:1557:HOH:O	2.20	0.48
1:D:473:ASP:CG	6:D:1538:HOH:O	2.52	0.48
1:A:74:ASN:ND2	1:A:352:LEU:HG	2.28	0.48
1:A:465:VAL:CG1	1:A:466:VAL:N	2.77	0.48
1:A:482:GLN:CB	6:A:1530:HOH:O	2.60	0.48
1:B:260:ARG:HB3	1:B:270:PHE:CE1	2.48	0.48
1:C:15:VAL:CG2	6:C:1687:HOH:O	2.62	0.48
1:C:74:ASN:HD21	1:C:83:ASN:HD22	1.60	0.48
1:D:141:ASN:HB2	6:D:1228:HOH:O	2.12	0.48
1:B:74:ASN:HD21	1:B:448:PRO:HG2	1.79	0.48
1:B:352:LEU:O	1:B:356:ILE:HG13	2.14	0.48
1:D:331:ASN:ND2	1:D:332:PHE:H	2.12	0.48
1:D:333:ASN:OD1	1:D:333:ASN:C	2.53	0.48
1:B:5:VAL:HG23	1:B:5:VAL:O	2.12	0.47
1:B:486:ASP:C	1:B:489:PRO:HD2	2.33	0.47
1:B:385:PRO:CD	1:B:436:ASN:OD1	2.62	0.47
1:B:135:ASP:OD2	6:B:1633:HOH:O	2.20	0.47
1:B:376:SER:HB3	1:B:470:ASP:HB2	1.96	0.47
2:B:611:NAG:C4	2:B:613:NAG:C1	2.91	0.47
1:D:486:ASP:C	1:D:489:PRO:HD2	2.35	0.47
1:A:59:LYS:HD3	1:A:499:GLN:C	2.34	0.47
1:A:498:ASP:CB	6:A:1586:HOH:O	2.63	0.47
1:B:497:SER:C	1:B:499:GLN:N	2.68	0.47
1:C:408:ARG:HD2	1:C:415:TYR:CZ	2.50	0.47
1:C:486:ASP:C	1:C:489:PRO:HD2	2.35	0.47
1:C:49:ILE:HD12	6:C:1242:HOH:O	2.14	0.47
2:D:805:NAG:C3	4:D:808:PYE:H22	2.44	0.47
1:B:223:THR:CG2	1:B:228:THR:OG1	2.63	0.47
1:D:314:PRO:HG2	1:D:440:ARG:HB3	1.95	0.47
1:A:374:LEU:HD22	1:A:467:PHE:HB3	1.97	0.47
1:A:497:SER:C	1:A:499:GLN:N	2.68	0.47
1:B:43:ARG:HG3	1:B:98:GLN:HG2	1.97	0.47
1:B:82:ILE:HG22	1:B:83:ASN:OD1	2.14	0.47
1:B:364:ASP:CG	6:B:1529:HOH:O	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASN:OD1	2:C:706:NAG:C1	2.62	0.47
1:C:74:ASN:HD21	1:C:448:PRO:HG2	1.79	0.47
1:C:352:LEU:HD13	1:C:484:TRP:CZ2	2.50	0.47
1:D:333:ASN:ND2	2:D:812:NAG:C1	2.78	0.47
1:D:380:ILE:HD11	1:D:443:THR:HG23	1.96	0.47
1:D:497:SER:C	1:D:499:GLN:N	2.68	0.47
1:B:345:THR:HG23	1:B:345:THR:O	2.15	0.47
1:C:201:VAL:HG13	1:C:243:ARG:CG	2.41	0.47
1:D:27:VAL:HG22	1:D:120:LEU:HD13	1.95	0.47
1:D:329:ALA:H	1:D:340:ASN:ND2	2.13	0.47
1:A:223:THR:CG2	1:A:228:THR:OG1	2.63	0.47
1:A:256:ASN:HB3	1:A:289:PRO:HG3	1.96	0.47
1:B:398:HIS:O	1:B:451:LEU:HD12	2.15	0.47
1:D:333:ASN:HD21	2:D:812:NAG:C1	2.28	0.47
1:D:345:THR:HG23	1:D:345:THR:O	2.15	0.47
1:A:2:ILE:N	6:A:1060:HOH:O	2.48	0.46
1:C:322:VAL:HG22	1:C:379:ASP:C	2.35	0.46
1:A:31:THR:O	1:A:32:PRO:C	2.52	0.46
1:A:191:THR:HG22	6:A:1216:HOH:O	2.14	0.46
1:A:499:GLN:HG2	6:A:1425:HOH:O	2.15	0.46
1:B:7:ASP:OD1	1:B:47:ASN:HB3	2.15	0.46
1:B:405:ALA:HB2	1:B:422:PHE:CZ	2.50	0.46
2:D:805:NAG:H2	2:D:806:NAG:O4	2.15	0.46
1:A:322:VAL:HG22	1:A:379:ASP:C	2.36	0.46
1:B:169:THR:OG1	1:B:275:ASN:ND2	2.48	0.46
1:C:494:ARG:NH2	6:C:1016:HOH:O	2.48	0.46
1:A:483:ALA:CA	6:A:1530:HOH:O	2.55	0.46
1:D:419:ASN:N	1:D:420:PRO:CD	2.79	0.46
1:B:315:GLY:HA2	6:B:1444:HOH:O	2.15	0.46
1:B:332:PHE:HZ	1:B:334:GLY:O	1.96	0.46
1:D:380:ILE:CD1	1:D:443:THR:HG23	2.45	0.46
1:A:149:VAL:HB	1:A:170:LEU:HB2	1.97	0.46
1:A:176:ARG:HG3	1:A:185:LEU:HD21	1.98	0.46
1:A:458:HIS:HE2	5:A:514:XYD:C6	2.29	0.46
1:A:486:ASP:C	1:A:489:PRO:HD2	2.35	0.46
1:C:497:SER:O	1:C:499:GLN:N	2.48	0.46
1:D:31:THR:O	1:D:32:PRO:C	2.50	0.46
1:C:352:LEU:O	1:C:356:ILE:HG13	2.15	0.46
1:D:7:ASP:OD1	1:D:47:ASN:HB3	2.15	0.46
1:D:149:VAL:HB	1:D:170:LEU:HB2	1.96	0.46
1:D:169:THR:OG1	1:D:275:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HD2	6:A:1368:HOH:O	2.14	0.46
1:B:280:ARG:CZ	1:B:286:ALA:HA	2.45	0.46
1:C:7:ASP:OD1	1:C:47:ASN:HB3	2.15	0.46
1:C:499:GLN:NE2	6:C:1008:HOH:O	2.42	0.46
1:D:408:ARG:HD2	1:D:415:TYR:CZ	2.51	0.46
1:A:7:ASP:OD1	1:A:47:ASN:HB3	2.15	0.46
1:A:37:THR:N	6:A:1060:HOH:O	2.33	0.46
1:A:191:THR:HG23	1:A:196:TYR:OH	2.16	0.46
1:A:495:ASP:HB2	1:A:498:ASP:HB2	1.98	0.46
1:B:318:VAL:HG13	6:B:1614:HOH:O	2.04	0.46
1:B:331:ASN:ND2	1:B:332:PHE:H	2.13	0.46
1:C:191:THR:HG23	1:C:196:TYR:OH	2.16	0.46
1:A:376:SER:HB3	1:A:470:ASP:HB2	1.98	0.46
1:B:31:THR:CG2	1:B:32:PRO:CD	2.93	0.46
1:C:301:ASN:HB3	1:C:304:ASN:ND2	2.31	0.46
1:D:57:MET:O	1:D:58:LEU:HB2	2.15	0.46
1:D:322:VAL:HG22	1:D:379:ASP:C	2.37	0.46
2:D:811:NAG:N2	2:D:812:NAG:O4	2.49	0.46
1:A:497:SER:O	1:A:499:GLN:N	2.50	0.45
1:B:2:ILE:O	1:B:3:GLY:O	2.34	0.45
1:B:374:LEU:HG	1:B:380:ILE:CD1	2.45	0.45
1:B:465:VAL:CG1	1:B:466:VAL:N	2.80	0.45
1:D:376:SER:HB3	1:D:470:ASP:HB2	1.97	0.45
1:A:158:LEU:HD12	2:A:505:NAG:O7	2.16	0.45
1:A:345:THR:HG23	1:A:345:THR:O	2.16	0.45
1:A:418:ASP:HA	6:A:1431:HOH:O	2.14	0.45
1:C:345:THR:HG23	1:C:345:THR:O	2.17	0.45
1:A:408:ARG:HD2	1:A:415:TYR:CZ	2.51	0.45
1:B:497:SER:O	1:B:499:GLN:N	2.50	0.45
1:C:465:VAL:CG1	1:C:466:VAL:N	2.79	0.45
1:D:465:VAL:CG1	1:D:466:VAL:N	2.78	0.45
1:B:155:ALA:N	2:B:605:NAG:H83	2.31	0.45
1:D:373:SER:O	1:D:374:LEU:HD12	2.16	0.45
1:D:380:ILE:O	1:D:440:ARG:HA	2.17	0.45
2:D:811:NAG:HN2	2:D:812:NAG:C4	2.29	0.45
1:A:31:THR:HG21	6:A:1494:HOH:O	1.93	0.45
1:A:233:VAL:HG13	1:A:234:ASP:N	2.32	0.45
1:C:405:ALA:HB2	1:C:422:PHE:CZ	2.52	0.45
1:D:330:PHE:HB2	1:D:387:THR:HG22	1.98	0.45
1:A:380:ILE:O	1:A:440:ARG:HA	2.17	0.45
1:C:377:ASN:CG	1:C:377:ASN:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:C	1:D:208:ASN:ND2	2.69	0.45
1:D:322:VAL:HG22	1:D:379:ASP:O	2.16	0.45
1:A:352:LEU:HD13	1:A:484:TRP:CZ2	2.52	0.45
1:B:101:ASP:CB	6:B:1133:HOH:O	2.65	0.45
1:B:144:THR:O	1:B:198:PHE:HA	2.17	0.45
1:B:374:LEU:HD22	1:B:467:PHE:HB3	1.99	0.45
1:D:374:LEU:HD22	1:D:467:PHE:HB3	1.98	0.45
1:B:74:ASN:ND2	1:B:448:PRO:HD2	2.31	0.45
1:B:233:VAL:HG13	1:B:234:ASP:N	2.32	0.45
1:B:329:ALA:H	1:B:340:ASN:ND2	2.15	0.45
1:B:374:LEU:HG	1:B:380:ILE:HD13	1.98	0.45
1:C:3:GLY:N	6:C:1137:HOH:O	2.49	0.45
1:C:380:ILE:O	1:C:440:ARG:HA	2.16	0.45
1:A:36:ILE:CG2	6:A:1590:HOH:O	2.33	0.45
1:A:498:ASP:O	1:A:499:GLN:C	2.55	0.45
1:B:75:TRP:HB2	1:B:484:TRP:CD1	2.52	0.45
1:B:176:ARG:HG3	1:B:185:LEU:HD21	1.99	0.45
1:B:191:THR:HG23	1:B:196:TYR:OH	2.17	0.45
1:C:169:THR:OG1	1:C:275:ASN:ND2	2.50	0.45
1:D:169:THR:HB	1:D:275:ASN:HD22	1.82	0.45
1:B:55:HIS:CE1	6:B:1488:HOH:O	2.69	0.44
1:B:348:THR:HG23	6:B:1514:HOH:O	2.15	0.44
1:C:373:SER:O	1:C:374:LEU:HD12	2.17	0.44
1:D:144:THR:O	1:D:198:PHE:HA	2.17	0.44
1:D:303:VAL:HG11	6:D:1706:HOH:O	2.17	0.44
1:B:408:ARG:HD2	1:B:415:TYR:CZ	2.52	0.44
1:B:419:ASN:N	1:B:420:PRO:CD	2.79	0.44
1:C:43:ARG:HE	1:C:45:GLN:CG	2.29	0.44
1:D:374:LEU:HG	1:D:380:ILE:CD1	2.47	0.44
1:B:322:VAL:HG22	1:B:379:ASP:CB	2.47	0.44
1:D:75:TRP:HB2	1:D:484:TRP:CD1	2.52	0.44
1:D:224:ASP:HB2	1:D:423:ARG:HB2	1.99	0.44
1:D:305:LEU:HB2	1:D:421:ILE:HG12	2.00	0.44
1:B:498:ASP:O	1:B:499:GLN:C	2.56	0.44
1:B:387:THR:O	1:B:389:ALA:N	2.51	0.44
1:C:495:ASP:HB2	1:C:498:ASP:HB2	1.99	0.44
1:D:226:ILE:N	1:D:226:ILE:HD12	2.33	0.44
1:A:66:HIS:O	1:A:106:PHE:HB3	2.18	0.44
1:C:5:VAL:O	1:C:5:VAL:HG23	2.17	0.44
1:C:144:THR:O	1:C:198:PHE:HA	2.17	0.44
1:C:223:THR:HB	1:C:244:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TRP:HB2	1:A:484:TRP:CD1	2.53	0.44
1:A:144:THR:O	1:A:198:PHE:HA	2.18	0.44
1:C:461:ALA:HA	6:C:1555:HOH:O	2.18	0.44
1:D:497:SER:O	1:D:499:GLN:N	2.50	0.44
1:A:446:PRO:N	6:A:1081:HOH:O	2.50	0.43
1:A:470:ASP:O	1:A:474:VAL:HG23	2.17	0.43
1:B:61:THR:OG1	1:B:115:GLN:NE2	2.51	0.43
1:C:419:ASN:N	1:C:420:PRO:CD	2.81	0.43
1:D:248:LEU:C	1:D:248:LEU:HD23	2.38	0.43
1:D:317:PRO:HA	1:D:417:TYR:CG	2.53	0.43
1:B:248:LEU:C	1:B:248:LEU:HD23	2.38	0.43
1:B:322:VAL:HG22	1:B:379:ASP:C	2.39	0.43
1:B:408:ARG:NH1	1:B:436:ASN:HB3	2.32	0.43
2:B:605:NAG:H5	4:B:616:PYE:C2	2.48	0.43
1:C:305:LEU:HB2	1:C:421:ILE:HG12	2.00	0.43
1:D:233:VAL:HG13	1:D:234:ASP:N	2.33	0.43
1:D:405:ALA:HB2	1:D:422:PHE:CZ	2.53	0.43
1:A:385:PRO:CD	1:A:436:ASN:OD1	2.66	0.43
1:A:405:ALA:HB2	1:A:422:PHE:CZ	2.53	0.43
1:B:305:LEU:HB2	1:B:421:ILE:HG12	2.00	0.43
1:B:338:PHE:HZ	2:B:610:NAG:HO6	1.66	0.43
1:D:380:ILE:HD11	1:D:443:THR:CG2	2.48	0.43
1:C:31:THR:O	1:C:32:PRO:C	2.54	0.43
1:D:498:ASP:O	1:D:499:GLN:C	2.56	0.43
1:A:155:ALA:H	2:A:505:NAG:H81	1.83	0.43
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.86	0.43
1:B:191:THR:HG23	6:B:1652:HOH:O	2.17	0.43
1:C:280:ARG:CZ	1:C:286:ALA:HA	2.48	0.43
1:D:11:THR:HB	6:D:1520:HOH:O	2.19	0.43
1:B:494:ARG:NH2	6:B:1011:HOH:O	2.52	0.43
1:C:461:ALA:C	6:C:1555:HOH:O	2.56	0.43
1:D:260:ARG:NE	1:D:293:GLN:HB2	2.33	0.43
1:B:380:ILE:HD11	1:B:443:THR:CG2	2.48	0.43
1:D:352:LEU:HD13	1:D:484:TRP:CZ2	2.54	0.43
2:D:805:NAG:C1	2:D:806:NAG:HO4	2.29	0.43
1:B:385:PRO:HG3	2:B:607:NAG:C1	2.49	0.43
1:D:280:ARG:CZ	1:D:286:ALA:HA	2.48	0.43
4:D:808:PYE:O5	4:D:810:PYE:H32	2.18	0.43
1:A:419:ASN:HD22	1:A:419:ASN:HA	1.59	0.43
2:B:605:NAG:H4	4:B:608:PYE:H21	1.99	0.43
1:C:113:SER:OG	6:C:1258:HOH:O	2.08	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:VAL:O	1:D:5:VAL:HG23	2.18	0.43
1:A:37:THR:C	6:A:1789:HOH:O	2.56	0.43
1:A:240:ALA:O	1:A:241:ALA:HB3	2.19	0.43
1:A:419:ASN:N	1:A:420:PRO:CD	2.81	0.43
1:D:320:GLY:N	6:D:1400:HOH:O	2.52	0.43
2:B:609:NAG:C1	2:B:610:NAG:O4	2.67	0.42
1:C:75:TRP:HB2	1:C:484:TRP:CD1	2.53	0.42
1:C:178:PRO:HB2	6:C:1762:HOH:O	2.19	0.42
1:B:260:ARG:NE	1:B:293:GLN:HB2	2.35	0.42
1:B:387:THR:C	1:B:389:ALA:N	2.72	0.42
1:C:62:SER:O	1:C:110:SER:HA	2.19	0.42
1:A:223:THR:HB	1:A:244:TYR:CE1	2.54	0.42
1:B:224:ASP:HB2	1:B:423:ARG:HB2	2.01	0.42
1:C:408:ARG:HD2	1:C:415:TYR:CE1	2.54	0.42
1:D:151:TRP:HB2	1:D:170:LEU:HD22	2.00	0.42
1:A:5:VAL:HG23	1:A:5:VAL:O	2.18	0.42
1:A:327:ASN:HD22	2:A:512:NAG:H5	1.83	0.42
2:A:505:NAG:O4	4:A:508:PYE:C1	2.68	0.42
1:C:168:ALA:HA	6:C:1450:HOH:O	2.18	0.42
1:C:223:THR:CG2	1:C:228:THR:OG1	2.67	0.42
1:D:71:LYS:HA	1:D:445:ASN:OD1	2.20	0.42
1:D:408:ARG:NH1	1:D:436:ASN:HB3	2.34	0.42
1:A:43:ARG:CD	6:A:1368:HOH:O	2.68	0.42
1:A:62:SER:O	1:A:110:SER:HA	2.19	0.42
1:A:408:ARG:NH1	1:A:436:ASN:HB3	2.34	0.42
1:C:55:HIS:NE2	6:C:1466:HOH:O	1.90	0.42
1:C:57:MET:O	1:C:58:LEU:HB2	2.19	0.42
1:C:374:LEU:HD22	1:C:467:PHE:HB3	2.01	0.42
1:C:436:ASN:ND2	2:C:707:NAG:O7	2.53	0.42
1:D:43:ARG:HG3	1:D:98:GLN:HG2	2.01	0.42
1:A:77:ASP:OD2	1:A:400:HIS:ND1	2.52	0.42
2:B:605:NAG:O5	2:B:606:NAG:O4	2.33	0.42
1:C:260:ARG:NE	1:C:293:GLN:HB2	2.35	0.42
1:D:176:ARG:HD3	1:D:181:THR:HA	2.02	0.42
1:A:176:ARG:HD3	1:A:181:THR:HA	2.02	0.42
1:A:205:CYS:SG	1:A:456:ASP:HB2	2.60	0.42
1:A:242:GLN:NE2	1:A:423:ARG:NH2	2.68	0.42
1:B:37:THR:HA	1:B:125:VAL:O	2.20	0.42
1:C:374:LEU:HG	1:C:380:ILE:CD1	2.50	0.42
1:D:307:PRO:HD3	1:D:421:ILE:HA	2.02	0.42
1:A:37:THR:HA	1:A:125:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:OG1	1:A:115:GLN:NE2	2.53	0.42
1:A:251:ASN:HA	6:A:1382:HOH:O	2.20	0.42
1:A:335:THR:OG1	1:A:336:ASN:ND2	2.53	0.42
1:B:226:ILE:N	1:B:226:ILE:HD12	2.34	0.42
1:D:374:LEU:HG	1:D:380:ILE:HD13	2.01	0.42
1:D:407:VAL:HG22	1:D:438:THR:O	2.20	0.42
1:C:387:THR:O	1:C:389:ALA:N	2.53	0.42
1:D:227:ASN:HB3	6:D:1070:HOH:O	2.20	0.42
1:A:155:ALA:HB2	2:A:506:NAG:C6	2.50	0.41
1:A:488:CYS:HB2	1:A:489:PRO:HD3	2.02	0.41
1:C:206:ASP:HB3	1:C:207:PRO:HD3	2.02	0.41
1:C:226:ILE:HD11	6:C:1339:HOH:O	2.20	0.41
1:C:374:LEU:HG	1:C:380:ILE:HD13	2.01	0.41
1:C:385:PRO:HG3	1:C:436:ASN:OD1	2.19	0.41
1:D:23:GLN:H	2:D:805:NAG:C8	2.33	0.41
1:D:470:ASP:O	1:D:474:VAL:HG23	2.19	0.41
1:A:322:VAL:HG22	1:A:379:ASP:CB	2.50	0.41
1:B:163:PRO:HG2	1:B:457:PHE:CZ	2.55	0.41
1:B:242:GLN:C	1:B:243:ARG:HD3	2.40	0.41
1:C:226:ILE:HD12	1:C:226:ILE:N	2.35	0.41
1:C:470:ASP:O	1:C:474:VAL:HG23	2.20	0.41
1:D:81:PHE:C	1:D:82:ILE:HD12	2.41	0.41
4:D:808:PYE:H42	4:D:810:PYE:H52	2.02	0.41
1:A:373:SER:O	1:A:374:LEU:HD12	2.20	0.41
1:B:208:ASN:ND2	1:B:208:ASN:C	2.74	0.41
1:B:317:PRO:HA	1:B:417:TYR:CG	2.54	0.41
1:C:248:LEU:C	1:C:248:LEU:HD23	2.41	0.41
1:C:498:ASP:O	1:C:499:GLN:C	2.58	0.41
1:D:367:PRO:HG2	1:D:370:SER:HB2	2.03	0.41
1:A:155:ALA:HB2	2:A:505:NAG:H81	2.01	0.41
1:A:364:ASP:OD1	6:A:1191:HOH:O	2.21	0.41
1:A:377:ASN:O	1:A:377:ASN:CG	2.57	0.41
1:B:307:PRO:HD3	1:B:421:ILE:HA	2.01	0.41
1:B:333:ASN:OD1	2:B:610:NAG:C1	2.69	0.41
1:B:387:THR:C	1:B:389:ALA:H	2.23	0.41
1:D:120:LEU:HD12	1:D:120:LEU:C	2.41	0.41
1:A:242:GLN:C	1:A:243:ARG:HD3	2.41	0.41
1:A:374:LEU:HG	1:A:380:ILE:HD13	2.02	0.41
1:B:139:VAL:HB	1:B:196:TYR:CD2	2.55	0.41
1:B:322:VAL:HG22	1:B:379:ASP:O	2.20	0.41
2:B:605:NAG:H3	4:B:616:PYE:H22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:PRO:O	1:D:499:GLN:HG2	2.21	0.41
1:A:91:HIS:HE1	6:A:1571:HOH:O	2.00	0.41
1:B:408:ARG:HD2	1:B:415:TYR:CE1	2.55	0.41
1:C:322:VAL:HG22	1:C:379:ASP:CB	2.51	0.41
1:A:233:VAL:CG1	1:A:234:ASP:N	2.82	0.41
1:A:317:PRO:HA	1:A:417:TYR:CG	2.54	0.41
1:C:317:PRO:HA	1:C:417:TYR:CG	2.55	0.41
1:C:345:THR:HA	1:C:346:PRO:HD3	1.95	0.41
1:D:206:ASP:CB	1:D:207:PRO:CD	2.89	0.41
1:D:233:VAL:CG1	1:D:234:ASP:N	2.83	0.41
1:D:234:ASP:OD2	1:D:297:THR:N	2.45	0.41
1:D:242:GLN:C	1:D:243:ARG:HD3	2.41	0.41
1:B:151:TRP:HB2	1:B:170:LEU:HD22	2.03	0.41
1:B:233:VAL:CG1	1:B:234:ASP:N	2.83	0.41
1:C:408:ARG:NH1	1:C:436:ASN:HB3	2.36	0.41
1:D:398:HIS:O	1:D:451:LEU:HD12	2.20	0.41
1:D:488:CYS:HB2	1:D:489:PRO:HD3	2.01	0.41
1:A:224:ASP:HB2	1:A:423:ARG:HB2	2.03	0.41
1:A:280:ARG:CZ	1:A:286:ALA:HA	2.50	0.41
1:A:380:ILE:HD12	1:A:441:PHE:CE2	2.56	0.41
1:A:496:PRO:O	1:A:499:GLN:HG2	2.21	0.41
1:B:5:VAL:O	1:B:5:VAL:CG2	2.68	0.41
1:C:81:PHE:C	1:C:82:ILE:HD12	2.41	0.41
1:C:82:ILE:N	1:C:82:ILE:HD12	2.35	0.41
1:C:459:LEU:HD13	6:C:1053:HOH:O	2.21	0.41
1:D:206:ASP:CG	1:D:265:PHE:HZ	2.24	0.41
1:D:376:SER:HB3	1:D:470:ASP:CG	2.41	0.41
1:A:226:ILE:HD12	1:A:226:ILE:N	2.35	0.41
1:A:260:ARG:NE	1:A:293:GLN:HB2	2.36	0.41
1:B:62:SER:O	1:B:110:SER:HA	2.21	0.41
1:B:223:THR:HB	1:B:244:TYR:CE1	2.56	0.41
1:C:25:VAL:HG13	1:C:52:LEU:HD21	2.03	0.41
1:C:26:VAL:HG22	1:C:31:THR:N	2.36	0.41
1:D:186:SER:HA	6:D:1061:HOH:O	2.21	0.41
1:A:26:VAL:HG22	1:A:31:THR:N	2.36	0.40
1:A:82:ILE:N	1:A:82:ILE:HD12	2.36	0.40
1:B:318:VAL:HG12	1:B:319:ALA:N	2.36	0.40
1:C:419:ASN:HD22	1:C:419:ASN:HA	1.58	0.40
2:C:707:NAG:H61	2:C:708:NAG:C7	2.50	0.40
1:D:77:ASP:OD2	1:D:400:HIS:ND1	2.53	0.40
1:D:322:VAL:HG22	1:D:379:ASP:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:NE2	1:A:95:TYR:OH	2.43	0.40
1:A:407:VAL:HG22	1:A:438:THR:O	2.21	0.40
1:B:55:HIS:HA	1:B:59:LYS:HG3	2.04	0.40
1:B:176:ARG:HD3	1:B:181:THR:HA	2.03	0.40
1:C:242:GLN:HG2	1:C:425:VAL:HB	2.04	0.40
1:C:307:PRO:HD3	1:C:421:ILE:HA	2.03	0.40
1:C:314:PRO:HG2	1:C:440:ARG:HB3	2.02	0.40
1:D:408:ARG:HD2	1:D:415:TYR:CE1	2.56	0.40
1:B:333:ASN:OD1	1:B:333:ASN:C	2.59	0.40
1:A:208:ASN:ND2	1:A:208:ASN:C	2.75	0.40
1:B:25:VAL:HG13	1:B:52:LEU:HD21	2.03	0.40
1:C:376:SER:HB3	1:C:470:ASP:CG	2.42	0.40
1:D:377:ASN:O	1:D:377:ASN:CG	2.60	0.40
1:A:109:HIS:HB2	1:A:116:TYR:HB2	2.04	0.40
1:A:151:TRP:HB2	1:A:170:LEU:HD22	2.03	0.40
1:A:305:LEU:HB2	1:A:421:ILE:HG12	2.04	0.40
1:B:470:ASP:O	1:B:474:VAL:HG23	2.21	0.40
1:C:43:ARG:NE	1:C:45:GLN:CD	2.64	0.40
1:C:151:TRP:HB2	1:C:170:LEU:HD22	2.02	0.40
1:D:242:GLN:HG2	1:D:425:VAL:HB	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1560:HOH:O	6:A:1705:HOH:O[2_556]	1.63	0.57
6:A:1584:HOH:O	6:C:1103:HOH:O[2_646]	2.17	0.03
6:A:1491:HOH:O	6:B:1592:HOH:O[2_646]	2.19	0.01

## 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	497/499 (100%)	461 (93%)	30 (6%)	6 (1%)	13	19
1	B	497/499 (100%)	463 (93%)	27 (5%)	7 (1%)	11	15
1	C	497/499 (100%)	460 (93%)	30 (6%)	7 (1%)	11	15
1	D	497/499 (100%)	466 (94%)	25 (5%)	6 (1%)	13	19
All	All	1988/1996 (100%)	1850 (93%)	112 (6%)	26 (1%)	12	17

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLY
1	B	3	GLY
1	C	3	GLY
1	D	3	GLY
1	A	498	ASP
1	B	206	ASP
1	B	498	ASP
1	C	206	ASP
1	C	498	ASP
1	D	498	ASP
1	A	206	ASP
1	B	59	LYS
1	D	206	ASP
1	C	321	GLY
1	A	100	PRO
1	A	321	GLY
1	B	32	PRO
1	C	32	PRO
1	C	388	ALA
1	B	321	GLY
1	A	419	ASN
1	B	419	ASN
1	C	419	ASN
1	D	321	GLY
1	D	419	ASN
1	D	32	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	402/407 (99%)	375 (93%)	27 (7%)	16	26
1	B	402/407 (99%)	379 (94%)	23 (6%)	20	33
1	C	402/407 (99%)	379 (94%)	23 (6%)	20	33
1	D	402/407 (99%)	379 (94%)	23 (6%)	20	33
All	All	1608/1628 (99%)	1512 (94%)	96 (6%)	19	31

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	26	VAL
1	A	100	PRO
1	A	116	TYR
1	A	120	LEU
1	A	124	PHE
1	A	205	CYS
1	A	207	PRO
1	A	208	ASN
1	A	223	THR
1	A	233	VAL
1	A	234	ASP
1	A	322	VAL
1	A	324	LEU
1	A	331	ASN
1	A	348	THR
1	A	352	LEU
1	A	399	LEU
1	A	419	ASN
1	A	421	ILE
1	A	431	PRO
1	A	450	PHE
1	A	456	ASP
1	A	459	LEU
1	A	463	PHE
1	A	487	LEU
1	A	490	THR
1	B	22	ARG
1	B	26	VAL
1	B	116	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	120	LEU
1	B	124	PHE
1	B	208	ASN
1	B	223	THR
1	B	233	VAL
1	B	234	ASP
1	B	322	VAL
1	B	324	LEU
1	B	331	ASN
1	B	348	THR
1	B	352	LEU
1	B	399	LEU
1	B	419	ASN
1	B	421	ILE
1	B	450	PHE
1	B	456	ASP
1	B	459	LEU
1	B	463	PHE
1	B	487	LEU
1	B	490	THR
1	C	22	ARG
1	C	43	ARG
1	C	116	TYR
1	C	120	LEU
1	C	124	PHE
1	C	208	ASN
1	C	223	THR
1	C	233	VAL
1	C	234	ASP
1	C	322	VAL
1	C	324	LEU
1	C	331	ASN
1	C	348	THR
1	C	352	LEU
1	C	385	PRO
1	C	399	LEU
1	C	419	ASN
1	C	421	ILE
1	C	450	PHE
1	C	459	LEU
1	C	463	PHE
1	C	487	LEU

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Mol	Chain	Res	Type
1	C	490	THR
1	D	22	ARG
1	D	26	VAL
1	D	116	TYR
1	D	120	LEU
1	D	124	PHE
1	D	208	ASN
1	D	223	THR
1	D	233	VAL
1	D	234	ASP
1	D	322	VAL
1	D	324	LEU
1	D	331	ASN
1	D	348	THR
1	D	352	LEU
1	D	399	LEU
1	D	419	ASN
1	D	421	ILE
1	D	450	PHE
1	D	456	ASP
1	D	459	LEU
1	D	463	PHE
1	D	487	LEU
1	D	490	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	70	GLN
1	A	74	ASN
1	A	84	GLN
1	A	98	GLN
1	A	115	GLN
1	A	208	ASN
1	A	217	ASN
1	A	237	GLN
1	A	275	ASN
1	A	304	ASN
1	A	306	HIS
1	A	327	ASN
1	A	331	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	333	ASN
1	A	336	ASN
1	A	340	ASN
1	A	360	GLN
1	A	361	ASN
1	A	419	ASN
1	A	436	ASN
1	A	478	ASN
1	B	54	ASN
1	B	70	GLN
1	B	74	ASN
1	B	84	GLN
1	B	115	GLN
1	B	208	ASN
1	B	237	GLN
1	B	275	ASN
1	B	304	ASN
1	B	306	HIS
1	B	327	ASN
1	B	331	ASN
1	B	336	ASN
1	B	340	ASN
1	B	360	GLN
1	B	361	ASN
1	B	419	ASN
1	B	478	ASN
1	C	54	ASN
1	C	70	GLN
1	C	74	ASN
1	C	84	GLN
1	C	115	GLN
1	C	208	ASN
1	C	217	ASN
1	C	237	GLN
1	C	275	ASN
1	C	304	ASN
1	C	306	HIS
1	C	327	ASN
1	C	331	ASN
1	C	336	ASN
1	C	340	ASN
1	C	360	GLN

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Mol	Chain	Res	Type
1	C	361	ASN
1	C	419	ASN
1	C	436	ASN
1	C	478	ASN
1	C	499	GLN
1	D	54	ASN
1	D	70	GLN
1	D	74	ASN
1	D	84	GLN
1	D	115	GLN
1	D	208	ASN
1	D	217	ASN
1	D	237	GLN
1	D	275	ASN
1	D	304	ASN
1	D	306	HIS
1	D	327	ASN
1	D	331	ASN
1	D	333	ASN
1	D	336	ASN
1	D	340	ASN
1	D	360	GLN
1	D	361	ASN
1	D	419	ASN
1	D	436	ASN
1	D	478	ASN

### 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

Of 56 ligands modelled in this entry, 16 are monoatomic - leaving 40 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
2	NAG	C	705	-	14,14,15	0.74	0	17,19,21	0.80	1 (5%)
2	NAG	A	507	-	14,14,15	0.50	0	17,19,21	0.62	0
2	NAG	C	707	-	14,14,15	0.49	0	17,19,21	0.77	1 (5%)
2	NAG	A	511	-	14,14,15	0.48	0	17,19,21	0.73	1 (5%)
5	XYD	C	712	-	9,9,9	6.07	6 (66%)	12,12,12	3.03	3 (25%)
5	XYD	D	814	-	9,9,9	6.36	6 (66%)	12,12,12	2.67	2 (16%)
4	PYE	D	809	-	6,6,6	0.90	0	6,6,6	0.44	0
4	PYE	A	508	-	6,6,6	0.77	0	6,6,6	0.42	0
4	PYE	B	615	-	6,6,6	0.81	0	6,6,6	0.41	0
4	PYE	B	608	-	6,6,6	0.76	0	6,6,6	0.47	0
2	NAG	A	510	-	14,14,15	0.60	0	17,19,21	0.67	0
2	NAG	D	811	-	14,14,15	0.50	0	17,19,21	0.69	1 (5%)
2	NAG	D	806	-	14,14,15	0.71	0	17,19,21	0.78	0
2	NAG	B	610	-	14,14,15	0.55	0	17,19,21	0.65	1 (5%)
2	NAG	B	613	-	14,14,15	0.50	0	17,19,21	0.73	0
2	NAG	D	805	-	14,14,15	0.55	0	17,19,21	0.84	1 (5%)
2	NAG	A	512	-	14,14,15	0.41	0	17,19,21	0.72	0
2	NAG	A	505	-	14,14,15	0.47	0	17,19,21	0.83	0
2	NAG	A	513	-	14,14,15	0.62	0	17,19,21	0.88	1 (5%)
4	PYE	B	614	-	6,6,6	0.85	0	6,6,6	0.40	0
4	PYE	D	808	-	6,6,6	0.80	0	6,6,6	0.55	0
2	NAG	C	706	-	14,14,15	0.55	0	17,19,21	0.69	0
2	NAG	B	607	-	14,14,15	0.64	0	17,19,21	0.66	1 (5%)
2	NAG	B	611	-	14,14,15	0.47	0	17,19,21	0.64	0
5	XYD	A	514	-	9,9,9	6.30	5 (55%)	12,12,12	2.75	3 (25%)
4	PYE	A	509	-	6,6,6	0.75	0	6,6,6	0.46	0
2	NAG	D	813	-	14,14,15	0.49	0	17,19,21	0.62	0
4	PYE	D	810	-	6,6,6	0.87	0	6,6,6	0.41	0
2	NAG	B	605	-	14,14,15	0.59	0	17,19,21	0.56	0
2	NAG	C	711	-	14,14,15	0.61	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	XYD	B	612	-	9,9,9	6.27	6 (66%)	12,12,12	2.74	3 (25%)
2	NAG	C	709	-	14,14,15	0.57	0	17,19,21	0.53	0
2	NAG	C	708	-	14,14,15	0.45	0	17,19,21	0.70	1 (5%)
2	NAG	B	606	-	14,14,15	0.80	0	17,19,21	1.65	2 (11%)
4	PYE	B	616	-	6,6,6	0.78	0	6,6,6	0.43	0
2	NAG	A	506	-	14,14,15	0.62	0	17,19,21	0.82	0
2	NAG	D	807	-	14,14,15	0.54	0	17,19,21	0.72	1 (5%)
2	NAG	D	812	-	14,14,15	0.57	0	17,19,21	0.62	0
2	NAG	C	710	-	14,14,15	0.48	0	17,19,21	0.73	1 (5%)
2	NAG	B	609	-	14,14,15	0.54	0	17,19,21	0.98	1 (5%)

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	C	705	-	-	5/6/23/26	0/1/1/1
2	NAG	A	507	-	-	3/6/23/26	0/1/1/1
2	NAG	C	707	-	-	2/6/23/26	0/1/1/1
2	NAG	A	511	-	-	4/6/23/26	0/1/1/1
5	XYD	C	712	-	-	-	0/1/1/1
5	XYD	D	814	-	-	-	0/1/1/1
4	PYE	D	809	-	-	-	0/1/1/1
4	PYE	A	508	-	-	-	0/1/1/1
4	PYE	B	615	-	-	-	0/1/1/1
4	PYE	B	608	-	-	-	0/1/1/1
2	NAG	A	510	-	-	2/6/23/26	0/1/1/1
2	NAG	D	811	-	-	2/6/23/26	0/1/1/1
2	NAG	D	806	-	-	0/6/23/26	0/1/1/1
2	NAG	B	610	-	-	4/6/23/26	0/1/1/1
2	NAG	B	613	-	-	3/6/23/26	0/1/1/1
2	NAG	D	805	-	-	2/6/23/26	0/1/1/1
2	NAG	A	512	-	-	4/6/23/26	0/1/1/1
2	NAG	A	505	-	-	4/6/23/26	0/1/1/1
2	NAG	A	513	-	-	2/6/23/26	0/1/1/1
4	PYE	B	614	-	-	-	0/1/1/1
4	PYE	D	808	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	706	-	-	2/6/23/26	0/1/1/1
2	NAG	B	607	-	-	2/6/23/26	0/1/1/1
2	NAG	B	611	-	-	4/6/23/26	0/1/1/1
5	XYD	A	514	-	-	-	0/1/1/1
4	PYE	A	509	-	-	-	0/1/1/1
2	NAG	D	813	-	-	4/6/23/26	0/1/1/1
4	PYE	D	810	-	-	-	0/1/1/1
2	NAG	B	605	-	-	3/6/23/26	0/1/1/1
2	NAG	C	711	-	-	6/6/23/26	0/1/1/1
5	XYD	B	612	-	-	-	0/1/1/1
2	NAG	C	709	-	-	4/6/23/26	0/1/1/1
2	NAG	C	708	-	-	4/6/23/26	0/1/1/1
2	NAG	B	606	-	-	2/6/23/26	0/1/1/1
4	PYE	B	616	-	-	-	0/1/1/1
2	NAG	A	506	-	-	0/6/23/26	0/1/1/1
2	NAG	D	807	-	-	1/6/23/26	0/1/1/1
2	NAG	D	812	-	-	5/6/23/26	0/1/1/1
2	NAG	C	710	-	-	3/6/23/26	0/1/1/1
2	NAG	B	609	-	-	2/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	814	XYD	C6-C1	10.03	1.54	1.40
5	B	612	XYD	C6-C1	9.88	1.54	1.40
5	C	712	XYD	C6-C1	9.73	1.54	1.40
5	A	514	XYD	C6-C5	9.66	1.55	1.39
5	A	514	XYD	C6-C1	9.53	1.54	1.40
5	D	814	XYD	C6-C5	9.49	1.54	1.39
5	B	612	XYD	C6-C5	9.04	1.54	1.39
5	C	712	XYD	C6-C5	8.87	1.53	1.39
5	A	514	XYD	C4-C3	8.27	1.53	1.38
5	D	814	XYD	C4-C3	8.23	1.53	1.38
5	B	612	XYD	C4-C3	8.21	1.53	1.38
5	D	814	XYD	C3-C2	8.06	1.57	1.39
5	B	612	XYD	C3-C2	7.95	1.56	1.39
5	A	514	XYD	C3-C2	7.89	1.56	1.39
5	C	712	XYD	C4-C3	7.86	1.53	1.38
5	C	712	XYD	C3-C2	7.55	1.55	1.39
5	B	612	XYD	C4-C5	5.89	1.55	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	514	XYD	C4-C5	5.86	1.55	1.38
5	D	814	XYD	C4-C5	5.61	1.54	1.38
5	C	712	XYD	C4-C5	5.56	1.54	1.38
5	B	612	XYD	C1-C2	2.47	1.57	1.42
5	D	814	XYD	C1-C2	2.39	1.57	1.42
5	C	712	XYD	C1-C2	2.30	1.56	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	712	XYD	C1-C6-C5	-9.41	117.99	122.18
5	A	514	XYD	C1-C6-C5	-8.51	118.39	122.18
5	B	612	XYD	C1-C6-C5	-8.40	118.44	122.18
5	D	814	XYD	C1-C6-C5	-8.15	118.55	122.18
2	B	606	NAG	C3-C4-C5	4.17	117.68	110.24
2	B	606	NAG	C6-C5-C4	-3.33	105.21	113.00
5	C	712	XYD	C4-C5-C6	2.64	121.93	117.95
5	A	514	XYD	C6-C1-C2	2.61	122.63	119.76
5	B	612	XYD	C4-C5-C6	2.56	121.81	117.95
5	D	814	XYD	C4-C5-C6	2.49	121.69	117.95
2	A	513	NAG	C2-N2-C7	-2.47	119.38	122.90
2	B	609	NAG	C2-N2-C7	-2.44	119.43	122.90
2	D	805	NAG	C4-C3-C2	-2.43	107.46	111.02
2	A	511	NAG	C2-N2-C7	-2.35	119.56	122.90
5	C	712	XYD	C6-C1-C2	2.32	122.31	119.76
2	B	610	NAG	C2-N2-C7	-2.24	119.71	122.90
2	D	811	NAG	C2-N2-C7	-2.22	119.75	122.90
2	C	710	NAG	C2-N2-C7	-2.19	119.79	122.90
2	C	708	NAG	C2-N2-C7	-2.16	119.83	122.90
2	C	707	NAG	C2-N2-C7	-2.10	119.91	122.90
2	D	807	NAG	C2-N2-C7	-2.07	119.96	122.90
5	A	514	XYD	C4-C5-C6	2.06	121.05	117.95
2	C	705	NAG	O5-C1-C2	-2.04	108.06	111.29
5	B	612	XYD	C6-C1-C2	2.02	121.98	119.76
2	B	607	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	507	NAG	C8-C7-N2-C2
2	A	507	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	510	NAG	C8-C7-N2-C2
2	A	510	NAG	O7-C7-N2-C2
2	A	511	NAG	C8-C7-N2-C2
2	A	511	NAG	O7-C7-N2-C2
2	A	512	NAG	C8-C7-N2-C2
2	A	512	NAG	O7-C7-N2-C2
2	A	513	NAG	C8-C7-N2-C2
2	A	513	NAG	O7-C7-N2-C2
2	B	605	NAG	C3-C2-N2-C7
2	B	607	NAG	C8-C7-N2-C2
2	B	607	NAG	O7-C7-N2-C2
2	B	609	NAG	C8-C7-N2-C2
2	B	609	NAG	O7-C7-N2-C2
2	B	611	NAG	C8-C7-N2-C2
2	B	611	NAG	O7-C7-N2-C2
2	B	613	NAG	C8-C7-N2-C2
2	B	613	NAG	O7-C7-N2-C2
2	C	705	NAG	C8-C7-N2-C2
2	C	705	NAG	O7-C7-N2-C2
2	C	708	NAG	C8-C7-N2-C2
2	C	708	NAG	O7-C7-N2-C2
2	C	709	NAG	C8-C7-N2-C2
2	C	709	NAG	O7-C7-N2-C2
2	C	710	NAG	C8-C7-N2-C2
2	C	710	NAG	O7-C7-N2-C2
2	C	711	NAG	C8-C7-N2-C2
2	C	711	NAG	O7-C7-N2-C2
2	D	805	NAG	C8-C7-N2-C2
2	D	805	NAG	O7-C7-N2-C2
2	D	812	NAG	C1-C2-N2-C7
2	D	812	NAG	C8-C7-N2-C2
2	D	812	NAG	O7-C7-N2-C2
2	D	813	NAG	C8-C7-N2-C2
2	D	813	NAG	O7-C7-N2-C2
2	B	605	NAG	C8-C7-N2-C2
2	B	610	NAG	C8-C7-N2-C2
2	B	610	NAG	O7-C7-N2-C2
2	B	613	NAG	C1-C2-N2-C7
2	B	611	NAG	O5-C5-C6-O6
2	B	605	NAG	O7-C7-N2-C2
2	D	811	NAG	C8-C7-N2-C2
2	C	711	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	505	NAG	O5-C5-C6-O6
2	C	709	NAG	C1-C2-N2-C7
2	C	711	NAG	C1-C2-N2-C7
2	D	813	NAG	C4-C5-C6-O6
2	B	611	NAG	C4-C5-C6-O6
2	D	811	NAG	O7-C7-N2-C2
2	A	505	NAG	C4-C5-C6-O6
2	B	610	NAG	O5-C5-C6-O6
2	D	813	NAG	O5-C5-C6-O6
2	A	511	NAG	O5-C5-C6-O6
2	A	512	NAG	O5-C5-C6-O6
2	B	610	NAG	C4-C5-C6-O6
2	C	708	NAG	O5-C5-C6-O6
2	A	512	NAG	C4-C5-C6-O6
2	C	705	NAG	C4-C5-C6-O6
2	A	507	NAG	C1-C2-N2-C7
2	A	505	NAG	C8-C7-N2-C2
2	C	705	NAG	O5-C5-C6-O6
2	C	709	NAG	O5-C5-C6-O6
2	C	707	NAG	C4-C5-C6-O6
2	D	812	NAG	C4-C5-C6-O6
2	C	705	NAG	C3-C2-N2-C7
2	C	711	NAG	C4-C5-C6-O6
2	D	812	NAG	O5-C5-C6-O6
2	C	707	NAG	O5-C5-C6-O6
2	A	505	NAG	O7-C7-N2-C2
2	B	606	NAG	C8-C7-N2-C2
2	C	706	NAG	C8-C7-N2-C2
2	C	708	NAG	C4-C5-C6-O6
2	B	606	NAG	O7-C7-N2-C2
2	C	711	NAG	C3-C2-N2-C7
2	D	807	NAG	O5-C5-C6-O6
2	C	706	NAG	O7-C7-N2-C2
2	A	511	NAG	C4-C5-C6-O6
2	C	710	NAG	C3-C2-N2-C7

There are no ring outliers.

38 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	705	NAG	4	0
2	A	507	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	707	NAG	8	0
5	C	712	XYD	2	0
5	D	814	XYD	3	0
4	D	809	PYE	2	0
4	A	508	PYE	4	0
4	B	615	PYE	2	0
4	B	608	PYE	9	0
2	A	510	NAG	4	0
2	D	811	NAG	3	0
2	D	806	NAG	7	0
2	B	610	NAG	4	0
2	B	613	NAG	2	0
2	D	805	NAG	8	0
2	A	512	NAG	11	0
2	A	505	NAG	9	0
2	A	513	NAG	2	0
4	B	614	PYE	4	0
4	D	808	PYE	10	0
2	C	706	NAG	7	0
2	B	607	NAG	4	0
2	B	611	NAG	3	0
5	A	514	XYD	4	0
4	A	509	PYE	2	0
4	D	810	PYE	4	0
2	B	605	NAG	10	0
2	C	711	NAG	3	0
5	B	612	XYD	3	0
2	C	709	NAG	1	0
2	C	708	NAG	3	0
2	B	606	NAG	7	0
4	B	616	PYE	5	0
2	A	506	NAG	9	0
2	D	807	NAG	3	0
2	D	812	NAG	5	0
2	C	710	NAG	1	0
2	B	609	NAG	1	0

## 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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.