



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:16 PM GMT

PDB ID : 1O7D  
Title : THE STRUCTURE OF THE BOVINE LYSOSOMAL A-MANNOSIDASE SUGGESTS A NOVEL MECHANISM FOR LOW PH ACTIVATION  
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Deposited on : 2002-10-30  
Resolution : 2.70 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

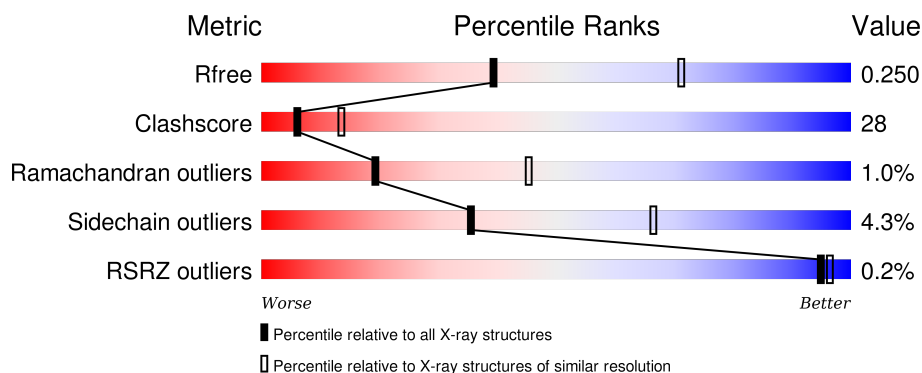
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*






The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	298	 58% 37% . .
2	B	84	 48% 38% 5% 10%
3	C	159	 51% 41% . 5%
4	D	282	 48% 46% . .
5	E	126	 48% 34% . 13%

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
7	TRS	A	2	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7385 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 LYSOSOMAL ALPHA-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	1
			2365	1520	408	426	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	GLY	ARG	CONFLICT SEE REMARK 9	UNP Q29451

- Molecule 2 is a protein called LYSOSOMAL ALPHA-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	1
			622	409	101	109	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	356	PRO	SER	CONFLICT SEE REMARK 9	UNP Q29451

- Molecule 3 is a protein called LYSOSOMAL ALPHA-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	151	Total	C	N	O	S	0	0	1
			1136	722	194	214	6			

- Molecule 4 is a protein called LYSOSOMAL ALPHA-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	270	Total	C	N	O	S	0	0	1
			2150	1356	397	392	5			

- Molecule 5 is a protein called LYSOSOMAL ALPHA-MANNOSIDASE.

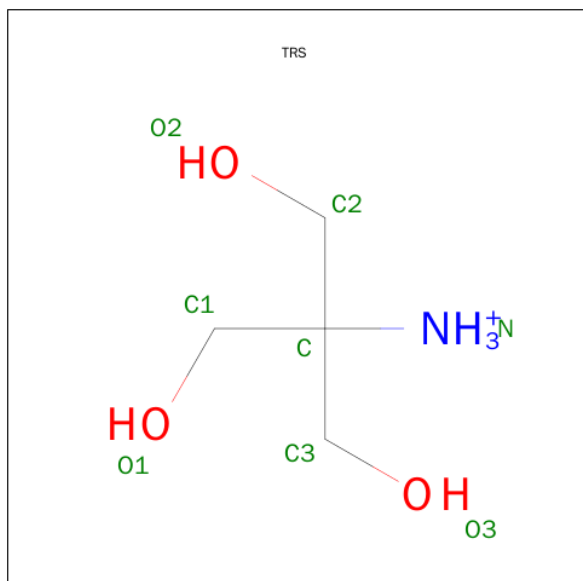
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	109	Total	C	N	O	S	0	0	1
			851	543	148	159	1			

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).

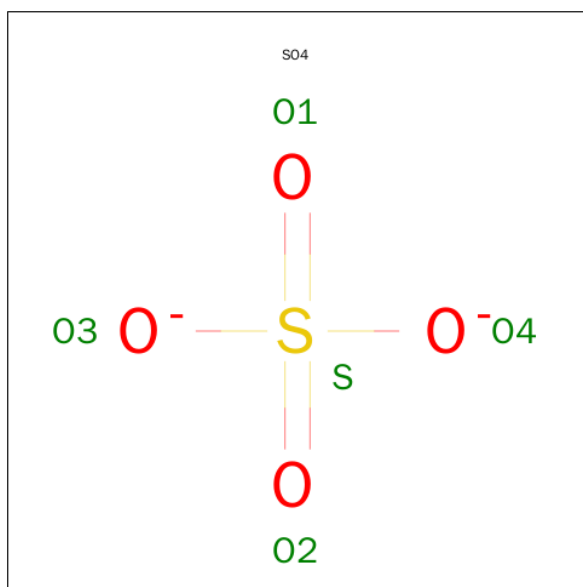


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 10 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	2	Total	C	N	O	0	0
			28	16	2	10		
12	D	2	Total	C	N	O	0	0
			28	16	2	10		

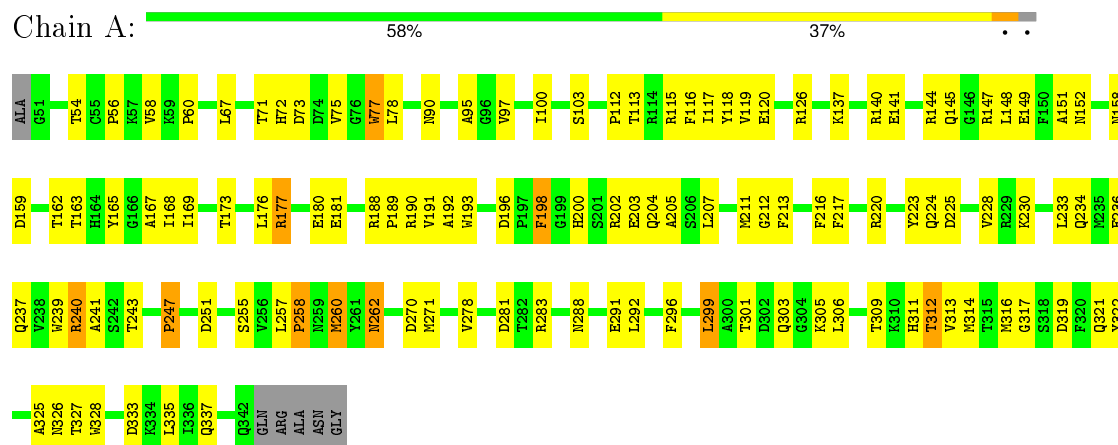
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	14	Total	O	0	0
			14	14		
13	B	2	Total	O	0	0
			2	2		
13	C	3	Total	O	0	0
			3	3		
13	D	14	Total	O	0	0
			14	14		
13	E	6	Total	O	0	0
			6	6		

### 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: LYSOSOMAL ALPHA-MANNOSIDASE







THR	P885	P886	T887	P888	P889	P890	P891	L905	A906	P907	P908	T912	L913	P916	L917	P918	P919	P920	P921	A922	P925	D926	P927	P928	P929	P930	L931	S932	T936	L937	D938	L939	T940	L941	P946	L951	P952	S953	P954	T955	L956	A957	A958	P967	T973	THR	GLY	PRO
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.88Å 117.88Å 582.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.62 – 2.51	Depositor EDS
% Data completeness (in resolution range)	89.4 (30.00-2.70) 86.0 (29.62-2.51)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.257 , 0.289 0.255 , 0.250	Depositor DCC
$R_{free}$ test set	3005 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	1 of 71690 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, NDG, SO4, TRS, MAN

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	0.46	0/2431	0.72	2/3302 (0.1%)
2	B	0.59	0/644	0.69	0/879
3	C	0.51	0/1163	0.72	0/1589
4	D	0.49	0/2198	0.74	0/2986
5	E	0.53	0/868	0.77	1/1186 (0.1%)
All	All	0.50	0/7304	0.73	3/9942 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	247	PRO	C-N-CD	-13.16	91.66	120.60
5	E	905	LEU	N-CA-C	-5.08	97.30	111.00
1	A	247	PRO	C-N-CA	5.05	143.23	122.00

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	2365	0	2290	129	0
2	B	622	0	587	48	0
3	C	1136	0	1106	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2150	0	2110	147	0
5	E	851	0	853	64	0
6	A	14	0	13	1	0
7	A	8	0	11	1	0
8	A	1	0	0	0	0
9	A	5	0	0	0	0
9	E	5	0	0	0	0
10	C	105	0	88	8	0
11	D	28	0	25	3	0
12	D	56	0	50	7	0
13	A	14	0	0	1	0
13	B	2	0	0	0	0
13	C	3	0	0	1	0
13	D	14	0	0	0	0
13	E	6	0	0	0	0
All	All	7385	0	7133	409	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 28.

All (409) 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)
3:C:540:PRO:CA	5:E:887:THR:HG21	1.81	1.10
1:A:237:GLN:NE2	2:B:373:LYS:HB2	1.69	1.07
3:C:540:PRO:HA	5:E:887:THR:HG21	1.12	1.06
2:B:403:ARG:HG3	2:B:403:ARG:HH11	1.14	1.02
4:D:748:ASN:HA	4:D:779:ASN:HD22	1.24	0.98
4:D:657:SER:HB3	4:D:817:LEU:HD23	1.49	0.94
1:A:167:ALA:HB1	3:C:444:GLN:NE2	1.82	0.94
1:A:237:GLN:HE21	2:B:373:LYS:HB2	1.35	0.90
1:A:119:VAL:HG22	1:A:151:ALA:HB3	1.52	0.89
1:A:167:ALA:HB1	3:C:444:GLN:HE21	1.35	0.88
4:D:717:GLY:HA2	4:D:837:TRP:HD1	1.39	0.88
10:C:1:NDG:H8C3	4:D:839:ARG:H	1.38	0.86
4:D:644:TYR:CZ	4:D:669:PRO:HG3	2.12	0.84
1:A:271:MET:SD	1:A:327:THR:HG21	2.17	0.84
5:E:954:THR:HG22	5:E:999:THR:HB	1.59	0.82
5:E:886:ARG:HG2	5:E:886:ARG:HH11	1.44	0.81
1:A:204:GLN:HE21	1:A:204:GLN:HA	1.44	0.81
3:C:540:PRO:HA	5:E:887:THR:CG2	2.05	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:OE2	1:A:144:ARG:NH2	2.11	0.80
3:C:585:ASN:N	13:C:2003:HOH:O	2.15	0.80
4:D:657:SER:HB3	4:D:817:LEU:CD2	2.12	0.79
3:C:564:LEU:HD23	3:C:565:LEU:N	1.98	0.78
3:C:488:GLU:HG2	4:D:873:GLN:O	1.81	0.78
4:D:716:VAL:HG21	4:D:813:VAL:HG11	1.66	0.78
4:D:714:TRP:CZ3	4:D:813:VAL:HG13	2.20	0.77
1:A:212:GLY:HA2	5:E:967:ARG:HD2	1.67	0.77
4:D:633:LEU:HD21	4:D:789:MET:HB2	1.66	0.77
1:A:303:GLN:HE21	1:A:312:THR:CG2	1.98	0.77
10:C:1:NDG:H8C2	4:D:839:ARG:HB3	1.67	0.76
4:D:755:ARG:HH11	4:D:755:ARG:HG2	1.50	0.76
3:C:440:MET:O	3:C:444:GLN:HG2	1.86	0.76
3:C:469:TRP:O	3:C:473:GLU:HG2	1.84	0.76
3:C:573:VAL:HG12	3:C:573:VAL:O	1.84	0.76
4:D:783:TYR:HB3	4:D:792:THR:HG23	1.68	0.76
1:A:71:THR:HG22	1:A:73:ASP:OD1	1.86	0.75
5:E:937:LEU:O	5:E:989:THR:HA	1.86	0.75
2:B:403:ARG:NH1	2:B:403:ARG:HG3	1.94	0.75
1:A:56:PRO:HG3	1:A:115:ARG:NH2	2.02	0.75
2:B:416:GLU:HB2	3:C:475:LEU:HD21	1.70	0.74
4:D:853:ALA:HB1	5:E:925:GLU:HB3	1.68	0.73
3:C:536:LEU:HD21	3:C:544:ILE:HG12	1.69	0.73
3:C:443:LEU:HD11	3:C:465:LEU:HG	1.69	0.72
2:B:383:GLY:O	2:B:386:MET:HG2	1.89	0.72
1:A:167:ALA:CB	3:C:444:GLN:NE2	2.52	0.72
4:D:686:VAL:HG12	4:D:687:GLN:N	2.05	0.72
3:C:522:VAL:CG1	3:C:524:TRP:HB2	2.19	0.72
5:E:886:ARG:HG2	5:E:886:ARG:NH1	2.02	0.71
4:D:627:GLU:HB2	4:D:634:LEU:HD12	1.72	0.71
4:D:644:TYR:CE1	4:D:669:PRO:HG3	2.26	0.71
3:C:444:GLN:HA	3:C:444:GLN:OE1	1.90	0.70
4:D:688:GLU:HB3	4:D:702:ARG:HG2	1.73	0.70
4:D:699:GLN:NE2	4:D:712:LEU:HD22	2.07	0.70
1:A:173:THR:O	1:A:177:ARG:HB2	1.92	0.70
3:C:472:CYS:O	3:C:476:MET:HG3	1.91	0.69
2:B:373:LYS:HE3	2:B:375:ASP:O	1.92	0.69
3:C:445:HIS:CD2	3:C:447:ASP:H	2.10	0.69
1:A:237:GLN:HE21	2:B:373:LYS:CB	2.04	0.69
3:C:539:ASP:HB2	3:C:540:PRO:CD	2.23	0.69
3:C:539:ASP:HB2	3:C:540:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HG2	1:A:251:ASP:OD1	1.93	0.69
4:D:716:VAL:CG2	4:D:813:VAL:HG11	2.23	0.68
1:A:317:GLY:HA2	1:A:321:GLN:OE1	1.92	0.68
4:D:861:GLU:HB3	5:E:901:ARG:NH2	2.09	0.68
1:A:204:GLN:NE2	1:A:204:GLN:HA	2.07	0.68
2:B:369:SER:OG	5:E:973:ASP:HB3	1.93	0.68
4:D:717:GLY:HA2	4:D:837:TRP:CD1	2.26	0.68
1:A:270:ASP:HB2	1:A:328:TRP:HE1	1.59	0.68
3:C:540:PRO:CB	5:E:887:THR:HG21	2.24	0.67
1:A:71:THR:HG23	1:A:321:GLN:H	1.59	0.67
10:C:1:NDG:H6C2	10:C:2:NAG:O5	1.93	0.67
10:C:1:NDG:C8	4:D:839:ARG:H	2.05	0.67
2:B:361:TRP:O	2:B:365:LYS:HG3	1.94	0.67
3:C:443:LEU:HD11	3:C:465:LEU:CG	2.24	0.67
4:D:817:LEU:HD12	4:D:817:LEU:N	2.11	0.66
3:C:525:MET:HE1	3:C:565:LEU:HB3	1.75	0.66
1:A:237:GLN:NE2	2:B:373:LYS:CB	2.55	0.66
2:B:411:VAL:HG22	3:C:517:PRO:HG3	1.76	0.66
1:A:278:VAL:HG22	1:A:292:LEU:HD11	1.78	0.66
4:D:737:LEU:HD11	4:D:784:ILE:HD12	1.77	0.65
4:D:695:ALA:CB	12:D:21:NAG:H83	2.27	0.65
3:C:513:ILE:HB	4:D:870:VAL:CG1	2.27	0.65
3:C:443:LEU:CD1	3:C:465:LEU:HD11	2.27	0.65
4:D:756:ARG:HB3	4:D:759:TYR:HB3	1.77	0.65
4:D:828:PRO:O	4:D:830:ASN:N	2.30	0.65
4:D:748:ASN:HA	4:D:779:ASN:ND2	2.05	0.64
3:C:527:ARG:HG3	3:C:565:LEU:HD11	1.78	0.64
4:D:647:SER:HB3	4:D:663:ARG:O	1.98	0.64
3:C:518:LEU:HD11	4:D:862:MET:HA	1.80	0.63
1:A:78:LEU:HD21	4:D:825:VAL:HA	1.80	0.63
4:D:750:ARG:NE	5:E:995:MET:HE1	2.14	0.63
1:A:303:GLN:HG2	1:A:312:THR:HG21	1.80	0.63
3:C:501:CYS:O	3:C:505:GLN:HG2	1.99	0.63
4:D:695:ALA:HB1	12:D:21:NAG:H83	1.81	0.63
4:D:612:LEU:HD11	4:D:708:ARG:O	1.99	0.63
1:A:240:ARG:HE	1:A:247:PRO:HG3	1.64	0.63
11:D:1:NAG:C6	11:D:11:NDG:C1	2.77	0.62
4:D:704:TYR:HB2	4:D:707:GLN:CD	2.19	0.62
1:A:97:VAL:HA	1:A:100:ILE:HD12	1.81	0.62
2:B:403:ARG:CG	2:B:403:ARG:HH11	2.00	0.62
1:A:278:VAL:HG22	1:A:292:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:686:VAL:HG22	4:D:704:TYR:CE1	2.34	0.62
5:E:907:ARG:HG3	5:E:907:ARG:HH11	1.64	0.62
1:A:58:VAL:O	1:A:60:PRO:HD3	2.00	0.61
1:A:234:GLN:NE2	2:B:371:SER:OG	2.34	0.61
1:A:213:PHE:O	5:E:967:ARG:NH1	2.34	0.60
1:A:117:ILE:HG13	1:A:117:ILE:O	2.00	0.60
5:E:954:THR:HG23	5:E:955:THR:O	2.01	0.60
1:A:112:PRO:HA	1:A:147:ARG:HH11	1.67	0.60
3:C:514:VAL:HG22	4:D:869:VAL:HG22	1.84	0.60
4:D:748:ASN:CA	4:D:779:ASN:HD22	2.08	0.60
3:C:443:LEU:HD11	3:C:465:LEU:CD1	2.31	0.59
1:A:203:GLU:OE1	4:D:750:ARG:HB2	2.00	0.59
3:C:564:LEU:O	3:C:565:LEU:HD12	2.03	0.59
4:D:737:LEU:O	4:D:737:LEU:HD12	2.02	0.59
4:D:809:LEU:HD23	4:D:810:GLU:N	2.18	0.59
4:D:692:ASN:ND2	12:D:2:NAG:H83	2.17	0.59
4:D:704:TYR:H	4:D:707:GLN:NE2	2.01	0.59
3:C:553:PRO:HD2	4:D:690:HIS:CE1	2.37	0.59
4:D:644:TYR:CZ	4:D:669:PRO:CG	2.86	0.58
2:B:359:TYR:O	2:B:363:LEU:HG	2.03	0.58
1:A:189:PRO:HB2	1:A:213:PHE:HE1	1.68	0.58
4:D:686:VAL:HG22	4:D:704:TYR:CD1	2.38	0.58
1:A:270:ASP:HB2	1:A:328:TRP:NE1	2.19	0.58
1:A:303:GLN:HE21	1:A:312:THR:HG21	1.68	0.58
1:A:141:GLU:O	1:A:145:GLN:HG2	2.02	0.58
1:A:223:TYR:CE2	2:B:384:PRO:HD3	2.38	0.58
3:C:582:GLN:O	3:C:582:GLN:HG3	2.03	0.58
5:E:919:HIS:ND1	5:E:994:PRO:HA	2.18	0.58
5:E:938:ASP:HA	5:E:988:ALA:O	2.03	0.58
3:C:484:SER:HA	5:E:886:ARG:HB3	1.86	0.57
4:D:611:TYR:O	4:D:612:LEU:HD23	2.04	0.57
4:D:721:VAL:CG1	4:D:816:ARG:HD3	2.34	0.57
1:A:159:ASP:HB2	3:C:446:HIS:HA	1.86	0.57
1:A:224:GLN:O	1:A:228:VAL:HG23	2.04	0.57
2:B:420:GLY:O	2:B:422:ALA:N	2.37	0.57
1:A:233:LEU:HD21	1:A:305:LYS:O	2.04	0.57
4:D:692:ASN:HD22	12:D:2:NAG:H83	1.70	0.57
4:D:709:HIS:HB3	4:D:845:LEU:CD2	2.34	0.57
3:C:513:ILE:N	3:C:513:ILE:HD12	2.19	0.56
4:D:745:THR:HG21	4:D:777:PRO:O	2.06	0.56
3:C:434:ALA:N	3:C:435:PRO:HD2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:THR:HG21	2:B:399:LYS:HE3	1.87	0.56
4:D:850:GLU:O	5:E:927:SER:HA	2.06	0.56
4:D:755:ARG:HD3	4:D:776:TYR:CG	2.42	0.55
11:D:1:NAG:H61	11:D:11:NDG:C1	2.36	0.55
4:D:854:ALA:CB	5:E:929:ARG:HH21	2.18	0.55
1:A:188:ARG:O	1:A:190:ARG:NH1	2.40	0.55
1:A:56:PRO:HD3	2:B:358:CYS:SG	2.47	0.55
1:A:112:PRO:HA	1:A:147:ARG:NH1	2.21	0.55
3:C:540:PRO:HB3	5:E:887:THR:CG2	2.37	0.55
3:C:527:ARG:HG2	3:C:563:GLU:OE1	2.07	0.55
3:C:540:PRO:CB	5:E:887:THR:CG2	2.85	0.55
4:D:794:LEU:HB2	4:D:843:LEU:HB2	1.88	0.55
3:C:553:PRO:HG2	4:D:690:HIS:CD2	2.42	0.55
1:A:240:ARG:HG3	1:A:240:ARG:HH11	1.71	0.55
4:D:692:ASN:HD22	12:D:2:NAG:C8	2.20	0.54
5:E:916:ARG:HG2	5:E:999:THR:HG23	1.88	0.54
4:D:755:ARG:HG2	4:D:755:ARG:NH1	2.19	0.54
4:D:682:LYS:HE3	4:D:687:GLN:NE2	2.22	0.54
4:D:625:GLU:CD	4:D:634:LEU:HD11	2.28	0.54
1:A:119:VAL:HG21	1:A:193:TRP:CD1	2.43	0.54
3:C:522:VAL:HG11	3:C:524:TRP:HB2	1.90	0.54
1:A:313:VAL:HG22	1:A:314:MET:N	2.23	0.54
1:A:220:ARG:NH1	1:A:260:MET:CE	2.71	0.54
4:D:686:VAL:CG1	4:D:687:GLN:N	2.71	0.53
5:E:907:ARG:HG3	5:E:907:ARG:NH1	2.22	0.53
4:D:658:GLY:N	4:D:817:LEU:HD22	2.24	0.53
1:A:243:THR:O	1:A:243:THR:HG22	2.07	0.53
4:D:660:TYR:CE2	4:D:825:VAL:HG23	2.43	0.53
4:D:774:ASN:O	4:D:802:SER:CB	2.56	0.53
4:D:653:SER:OG	4:D:663:ARG:NH1	2.41	0.53
4:D:854:ALA:HA	5:E:921:PHE:HE1	1.73	0.53
3:C:513:ILE:HB	4:D:870:VAL:HG13	1.90	0.53
2:B:400:ARG:HB2	4:D:797:ARG:CZ	2.38	0.53
3:C:539:ASP:HA	3:C:578:TYR:CD2	2.43	0.53
5:E:918:GLU:HB2	5:E:997:ILE:HG12	1.90	0.53
5:E:932:SER:O	5:E:994:PRO:HG3	2.08	0.53
4:D:854:ALA:HB1	5:E:929:ARG:HH21	1.74	0.53
5:E:951:LEU:HD12	5:E:1002:ALA:HB2	1.90	0.53
1:A:240:ARG:CG	1:A:251:ASP:OD1	2.57	0.53
1:A:314:MET:HB3	1:A:316:MET:CE	2.39	0.53
1:A:257:LEU:CD2	1:A:313:VAL:HG11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:527:ARG:HG3	3:C:565:LEU:CD1	2.39	0.52
1:A:314:MET:HB3	1:A:316:MET:HE1	1.90	0.52
4:D:616:PHE:CE1	4:D:689:VAL:HG21	2.45	0.52
4:D:817:LEU:HD12	4:D:817:LEU:H	1.73	0.52
5:E:886:ARG:HH11	5:E:886:ARG:CG	2.18	0.52
1:A:321:GLN:O	1:A:322:TYR:HB2	2.09	0.52
1:A:71:THR:HG23	1:A:321:GLN:N	2.24	0.52
6:A:1:NAG:C7	6:A:1:NAG:O3	2.58	0.52
4:D:721:VAL:HG13	4:D:816:ARG:HD3	1.91	0.52
1:A:335:LEU:C	1:A:335:LEU:HD13	2.29	0.52
2:B:381:ALA:HB2	2:B:387:PHE:CD1	2.45	0.52
4:D:784:ILE:HG13	4:D:784:ILE:O	2.10	0.52
1:A:230:LYS:HD2	1:A:306:LEU:HD13	1.92	0.52
3:C:488:GLU:N	3:C:488:GLU:OE1	2.42	0.51
3:C:457:VAL:HG12	3:C:461:TYR:CE2	2.46	0.51
1:A:220:ARG:CZ	1:A:260:MET:HE3	2.40	0.51
4:D:822:ALA:O	4:D:823:ARG:HD3	2.10	0.51
1:A:220:ARG:NH1	1:A:260:MET:HE1	2.26	0.51
1:A:54:THR:O	1:A:54:THR:HG22	2.09	0.51
4:D:716:VAL:HG21	4:D:813:VAL:CG1	2.39	0.51
4:D:692:ASN:ND2	12:D:2:NAG:C8	2.74	0.51
1:A:230:LYS:HB3	1:A:306:LEU:HD22	1.93	0.51
5:E:889:PHE:CG	5:E:890:SER:N	2.78	0.51
1:A:117:ILE:HA	1:A:149:GLU:O	2.11	0.51
1:A:223:TYR:CZ	2:B:384:PRO:HD3	2.46	0.51
4:D:774:ASN:O	4:D:802:SER:HB2	2.11	0.51
4:D:610:GLU:H	4:D:610:GLU:CD	2.13	0.51
3:C:495:LYS:C	3:C:497:ASN:N	2.61	0.51
2:B:386:MET:HB3	4:D:655:GLN:HG2	1.91	0.51
1:A:198:PHE:CD2	1:A:198:PHE:N	2.76	0.51
3:C:522:VAL:HG12	3:C:524:TRP:HB2	1.92	0.51
1:A:240:ARG:NH2	1:A:247:PRO:HB3	2.26	0.50
5:E:900:VAL:HG12	5:E:901:ARG:N	2.24	0.50
1:A:309:THR:C	1:A:311:HIS:H	2.15	0.50
4:D:699:GLN:HE22	4:D:712:LEU:HD22	1.77	0.50
3:C:513:ILE:HB	4:D:870:VAL:HG12	1.93	0.50
1:A:243:THR:CG2	1:A:243:THR:O	2.58	0.50
3:C:473:GLU:HB2	3:C:492:PHE:CE1	2.46	0.50
3:C:507:ALA:HB3	3:C:510:PHE:HD2	1.77	0.50
5:E:926:ASP:CG	5:E:932:SER:HB2	2.31	0.50
4:D:709:HIS:CD2	4:D:843:LEU:HD22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HG2	1:A:260:MET:HE1	1.94	0.50
1:A:165:TYR:O	1:A:169:ILE:HG13	2.11	0.50
3:C:564:LEU:HD23	3:C:565:LEU:H	1.75	0.50
3:C:488:GLU:CG	4:D:873:GLN:O	2.57	0.50
1:A:56:PRO:HG3	1:A:115:ARG:HH22	1.73	0.50
3:C:518:LEU:CD1	4:D:862:MET:HG2	2.42	0.50
4:D:660:TYR:CE2	4:D:823:ARG:HB2	2.47	0.50
1:A:204:GLN:HE21	1:A:204:GLN:CA	2.10	0.49
3:C:443:LEU:CD2	3:C:461:TYR:HB3	2.42	0.49
3:C:504:THR:HG21	3:C:528:LEU:HD13	1.94	0.49
3:C:564:LEU:C	3:C:565:LEU:HD12	2.33	0.49
4:D:751:GLU:HG3	5:E:995:MET:HE2	1.92	0.49
4:D:709:HIS:HB3	4:D:845:LEU:HD23	1.93	0.49
1:A:196:ASP:O	1:A:220:ARG:HD2	2.11	0.49
5:E:899:SER:HA	5:E:921:PHE:CE2	2.46	0.49
4:D:607:ILE:HG21	4:D:689:VAL:HG23	1.95	0.49
1:A:202:ARG:O	1:A:241:ALA:HB1	2.13	0.49
1:A:113:THR:HG22	2:B:353:TYR:HD2	1.78	0.49
4:D:744:TYR:CD1	4:D:744:TYR:N	2.80	0.49
4:D:866:ALA:HB1	4:D:867:PRO:HD2	1.95	0.49
1:A:237:GLN:HB2	2:B:371:SER:O	2.13	0.49
5:E:954:THR:CG2	5:E:958:ALA:HA	2.43	0.49
11:D:1:NAG:H61	11:D:11:NDG:O	2.13	0.49
1:A:291:GLU:OE1	1:A:291:GLU:HA	2.13	0.49
1:A:158:ASN:HA	3:C:444:GLN:O	2.13	0.49
4:D:780:SER:HB2	4:D:781:ARG:HE	1.78	0.49
2:B:395:ARG:HD2	3:C:451:GLY:HA2	1.95	0.48
1:A:224:GLN:HE22	4:D:766:ASN:HB3	1.78	0.48
1:A:314:MET:C	1:A:316:MET:HE3	2.33	0.48
1:A:56:PRO:HG3	1:A:115:ARG:CZ	2.42	0.48
5:E:900:VAL:CG1	5:E:901:ARG:N	2.77	0.48
3:C:443:LEU:HD11	3:C:465:LEU:HD11	1.91	0.48
2:B:396:PRO:HG2	4:D:814:HIS:CD2	2.49	0.48
4:D:805:ARG:HH11	4:D:805:ARG:HG3	1.78	0.48
4:D:607:ILE:O	4:D:607:ILE:HG13	2.12	0.48
2:B:411:VAL:HG22	3:C:517:PRO:CG	2.41	0.48
2:B:391:TYR:HA	2:B:394:SER:OG	2.14	0.48
1:A:240:ARG:HG3	1:A:240:ARG:NH1	2.29	0.47
4:D:732:ARG:HG3	4:D:809:LEU:O	2.14	0.47
2:B:403:ARG:NH1	2:B:403:ARG:CG	2.67	0.47
3:C:550:VAL:HG21	3:C:565:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:ALA:HB1	10:C:2:NAG:C8	2.45	0.47
2:B:414:GLN:O	2:B:418:LEU:HG	2.14	0.47
2:B:397:ALA:HB1	10:C:2:NAG:H82	1.96	0.47
1:A:54:THR:HG21	1:A:145:GLN:O	2.14	0.47
4:D:820:ASP:OD1	4:D:822:ALA:N	2.46	0.47
5:E:938:ASP:C	5:E:939:LEU:HD23	2.35	0.47
3:C:447:ASP:HA	3:C:452:THR:OG1	2.15	0.47
4:D:658:GLY:CA	4:D:817:LEU:HD22	2.44	0.47
4:D:635:LEU:HD13	4:D:789:MET:SD	2.54	0.47
3:C:537:VAL:HG22	3:C:580:VAL:HG22	1.96	0.47
1:A:288:ASN:O	1:A:292:LEU:HB2	2.15	0.47
1:A:126:ARG:HE	1:A:126:ARG:HB2	1.53	0.47
1:A:151:ALA:O	1:A:191:VAL:O	2.33	0.47
5:E:908:TRP:HB3	5:E:912:THR:HG22	1.97	0.47
4:D:667:ASN:ND2	4:D:770:PRO:CG	2.78	0.47
4:D:769:GLU:HB3	4:D:772:ALA:HB3	1.97	0.47
1:A:303:GLN:HE21	1:A:312:THR:HG22	1.76	0.46
5:E:939:LEU:HD23	5:E:939:LEU:N	2.30	0.46
1:A:72:HIS:HD2	1:A:319:ASP:OD1	1.98	0.46
5:E:918:GLU:CB	5:E:997:ILE:HG12	2.45	0.46
4:D:750:ARG:HE	5:E:995:MET:HE1	1.80	0.46
4:D:678:THR:HA	4:D:690:HIS:O	2.16	0.46
4:D:757:ARG:HH22	4:D:806:ASP:CG	2.18	0.46
1:A:119:VAL:HG13	1:A:152:ASN:CB	2.46	0.46
1:A:77:TRP:CE2	7:A:2:TRS:H12	2.51	0.46
3:C:520:ARG:CA	3:C:572:ALA:HB2	2.46	0.46
1:A:78:LEU:HD23	3:C:454:ARG:HG3	1.98	0.46
1:A:77:TRP:CD2	1:A:78:LEU:HG	2.51	0.46
5:E:940:THR:HG1	5:E:988:ALA:N	2.14	0.46
5:E:929:ARG:O	5:E:930:ASN:C	2.53	0.46
2:B:400:ARG:NH1	4:D:796:ASP:HB2	2.30	0.46
12:D:3:NAG:H61	12:D:31:NAG:C1	2.45	0.45
1:A:240:ARG:HH21	1:A:247:PRO:CG	2.29	0.45
2:B:414:GLN:HG2	5:E:905:LEU:HB3	1.98	0.45
4:D:723:ASP:CG	4:D:727:LYS:HZ1	2.20	0.45
1:A:335:LEU:HD13	1:A:335:LEU:O	2.17	0.45
4:D:644:TYR:CE2	4:D:669:PRO:HG3	2.50	0.45
4:D:686:VAL:CG2	4:D:704:TYR:CE1	2.99	0.45
1:A:223:TYR:HD1	2:B:381:ALA:O	2.00	0.45
1:A:202:ARG:CZ	4:D:753:LEU:HD21	2.46	0.45
5:E:954:THR:HG23	5:E:955:THR:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:814:HIS:CD2	4:D:815:ARG:H	2.35	0.45
1:A:200:HIS:H	2:B:377:PHE:HB2	1.82	0.45
5:E:936:THR:CG2	5:E:989:THR:CG2	2.95	0.45
3:C:539:ASP:HB3	3:C:545:VAL:HG21	1.99	0.45
2:B:369:SER:OG	5:E:973:ASP:CB	2.63	0.45
1:A:163:THR:OG1	1:A:168:ILE:HD11	2.17	0.44
3:C:465:LEU:O	3:C:469:TRP:HD1	2.00	0.44
3:C:431:GLY:O	3:C:475:LEU:HD13	2.18	0.44
4:D:703:LEU:HD23	4:D:703:LEU:HA	1.76	0.44
1:A:225:ASP:HB2	4:D:763:TRP:CZ3	2.52	0.44
4:D:774:ASN:O	4:D:802:SER:OG	2.31	0.44
4:D:730:ILE:HG13	4:D:730:ILE:O	2.17	0.44
1:A:176:LEU:O	1:A:180:GLU:HB2	2.17	0.44
2:B:403:ARG:NH2	4:D:779:ASN:O	2.50	0.44
4:D:854:ALA:HB1	5:E:929:ARG:NH2	2.32	0.44
5:E:953:GLU:HA	5:E:953:GLU:OE1	2.17	0.44
4:D:688:GLU:HA	4:D:701:VAL:O	2.17	0.44
4:D:817:LEU:C	4:D:818:LEU:HD23	2.38	0.44
4:D:699:GLN:HG2	4:D:700:VAL:N	2.33	0.44
1:A:301:THR:O	1:A:305:LYS:HG3	2.17	0.44
4:D:735:THR:N	4:D:807:GLY:O	2.50	0.44
3:C:486:LEU:HD11	3:C:511:GLN:NE2	2.32	0.44
5:E:946:PHE:HB3	5:E:1006:TRP:CD1	2.52	0.44
4:D:778:VAL:HG11	4:D:811:LEU:CD2	2.48	0.43
1:A:202:ARG:CG	1:A:241:ALA:HA	2.49	0.43
5:E:936:THR:HG23	5:E:989:THR:CG2	2.49	0.43
1:A:167:ALA:CB	3:C:444:GLN:HE22	2.27	0.43
4:D:750:ARG:NH1	5:E:997:ILE:HD11	2.33	0.43
1:A:103:SER:HB3	1:A:325:ALA:HB3	1.99	0.43
5:E:936:THR:CG2	5:E:989:THR:HG23	2.49	0.43
4:D:686:VAL:HG12	4:D:687:GLN:H	1.79	0.43
3:C:445:HIS:CG	3:C:446:HIS:N	2.86	0.43
1:A:240:ARG:HH21	1:A:247:PRO:CB	2.32	0.43
1:A:257:LEU:HD22	1:A:313:VAL:HG11	2.01	0.43
1:A:202:ARG:HA	1:A:239:TRP:CZ2	2.53	0.43
3:C:558:GLN:CD	3:C:558:GLN:N	2.72	0.43
4:D:605:LEU:HB3	4:D:616:PHE:HB2	2.01	0.43
4:D:728:GLU:OE2	4:D:815:ARG:NH2	2.49	0.43
4:D:660:TYR:CZ	4:D:825:VAL:HG23	2.54	0.43
1:A:137:LYS:HA	1:A:140:ARG:HH21	1.84	0.43
4:D:699:GLN:HE21	4:D:701:VAL:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:660:TYR:OH	4:D:825:VAL:HG23	2.19	0.42
5:E:926:ASP:OD1	5:E:932:SER:HB2	2.18	0.42
4:D:728:GLU:HG2	4:D:815:ARG:HB2	2.01	0.42
5:E:919:HIS:CE1	5:E:994:PRO:HA	2.54	0.42
4:D:617:ASP:HB3	4:D:620:THR:OG1	2.19	0.42
1:A:75:VAL:HG12	1:A:75:VAL:O	2.20	0.42
4:D:856:HIS:O	4:D:860:ALA:HB2	2.19	0.42
1:A:73:ASP:O	1:A:120:GLU:HG2	2.20	0.42
3:C:510:PHE:CE1	3:C:580:VAL:HB	2.53	0.42
1:A:177:ARG:O	1:A:181:GLU:HG2	2.19	0.42
3:C:528:LEU:HA	3:C:529:PRO:HD3	1.89	0.42
3:C:443:LEU:HD21	3:C:461:TYR:HB3	2.01	0.42
5:E:922:ALA:HA	5:E:995:MET:HG2	2.01	0.42
1:A:326:ASN:ND2	13:A:2013:HOH:O	2.51	0.42
2:B:403:ARG:O	2:B:403:ARG:HG2	2.20	0.42
4:D:838:VAL:HG12	4:D:839:ARG:N	2.34	0.42
3:C:445:HIS:CE1	3:C:446:HIS:CE1	3.08	0.42
5:E:899:SER:HA	5:E:921:PHE:HE2	1.85	0.42
5:E:906:ALA:O	5:E:913:LEU:HD22	2.19	0.42
2:B:406:TYR:CZ	2:B:410:GLN:NE2	2.87	0.42
2:B:406:TYR:OH	2:B:410:GLN:NE2	2.53	0.42
10:C:1:NDG:C8	4:D:839:ARG:N	2.81	0.42
4:D:851:THR:O	4:D:851:THR:HG22	2.20	0.42
3:C:575:PHE:CD1	3:C:575:PHE:C	2.93	0.42
1:A:257:LEU:HA	1:A:258:PRO:HD3	1.82	0.41
1:A:116:PHE:HE1	1:A:322:TYR:CE2	2.38	0.41
3:C:439:ALA:HB1	3:C:465:LEU:HD23	2.02	0.41
3:C:470:ARG:CB	3:C:471:PRO:HD3	2.50	0.41
3:C:545:VAL:HG13	3:C:546:PRO:HD2	2.01	0.41
5:E:940:THR:O	5:E:941:ASN:HB3	2.20	0.41
1:A:192:ALA:HB3	1:A:216:PHE:HD1	1.85	0.41
1:A:296:PHE:O	1:A:299:LEU:N	2.53	0.41
1:A:217:PHE:CD2	1:A:255:SER:HB3	2.55	0.41
5:E:887:THR:O	5:E:887:THR:HG22	2.20	0.41
4:D:723:ASP:OD2	4:D:727:LYS:NZ	2.47	0.41
1:A:90:ASN:ND2	1:A:95:ALA:H	2.18	0.41
1:A:118:TYR:HE2	1:A:120:GLU:O	2.04	0.41
2:B:416:GLU:CB	3:C:475:LEU:HD21	2.46	0.41
4:D:744:TYR:O	4:D:782:ILE:HA	2.20	0.41
3:C:538:LYS:HB2	3:C:579:SER:OG	2.20	0.41
1:A:167:ALA:CB	3:C:444:GLN:HE21	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:MET:HG2	5:E:956:LEU:HB3	2.03	0.41
4:D:609:ASN:C	4:D:609:ASN:OD1	2.59	0.41
3:C:524:TRP:CD2	4:D:867:PRO:HG3	2.55	0.41
1:A:281:ASP:OD1	1:A:283:ARG:HG3	2.21	0.41
1:A:67:LEU:HD23	1:A:314:MET:HB2	2.03	0.41
1:A:220:ARG:NH1	1:A:260:MET:HE3	2.36	0.41
1:A:205:ALA:HB3	1:A:241:ALA:HB2	2.03	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.72	0.41
1:A:262:ASN:N	1:A:262:ASN:ND2	2.69	0.41
4:D:714:TRP:CZ3	4:D:813:VAL:CG1	2.98	0.40
3:C:536:LEU:HD23	3:C:537:VAL:N	2.36	0.40
4:D:757:ARG:HG2	4:D:758:ASN:ND2	2.36	0.40
2:B:409:LEU:HD11	3:C:437:ASN:HA	2.02	0.40
3:C:509:ARG:HB3	4:D:875:GLY:N	2.36	0.40
4:D:685:LEU:O	4:D:705:PRO:HD3	2.21	0.40
4:D:704:TYR:O	4:D:707:GLN:HG2	2.21	0.40
2:B:397:ALA:CB	10:C:2:NAG:H82	2.51	0.40
5:E:954:THR:HG21	5:E:958:ALA:HA	2.03	0.40
4:D:611:TYR:CD1	4:D:611:TYR:N	2.88	0.40
2:B:387:PHE:O	4:D:661:ILE:HA	2.22	0.40
1:A:333:ASP:OD1	2:B:353:TYR:OH	2.31	0.40
1:A:200:HIS:HB2	2:B:377:PHE:CD2	2.56	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	290/298 (97%)	262 (90%)	25 (9%)	3 (1%)	19	45
2	B	74/84 (88%)	68 (92%)	5 (7%)	1 (1%)	14	35
3	C	149/159 (94%)	133 (89%)	15 (10%)	1 (1%)	26	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	266/282 (94%)	247 (93%)	16 (6%)	3 (1%)	17	42
5	E	105/126 (83%)	98 (93%)	6 (6%)	1 (1%)	19	45
All	All	884/949 (93%)	808 (91%)	67 (8%)	9 (1%)	19	45

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	920	GLN
1	A	77	TRP
2	B	421	PRO
4	D	874	GLY
1	A	260	MET
3	C	445	HIS
1	A	258	PRO
4	D	653	SER
4	D	829	LEU

### 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	251/260 (96%)	241 (96%)	10 (4%)	38	69
2	B	65/71 (92%)	59 (91%)	6 (9%)	11	25
3	C	125/139 (90%)	121 (97%)	4 (3%)	46	77
4	D	227/240 (95%)	218 (96%)	9 (4%)	38	69
5	E	93/111 (84%)	89 (96%)	4 (4%)	35	66
All	All	761/821 (93%)	728 (96%)	33 (4%)	35	66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	177	ARG

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Mol	Chain	Res	Type
1	A	198	PHE
1	A	207	LEU
1	A	236	GLU
1	A	240	ARG
1	A	262	ASN
1	A	299	LEU
1	A	312	THR
1	A	337	GLN
2	B	347	ILE
2	B	384	PRO
2	B	403	ARG
2	B	407	ASN
2	B	409	LEU
2	B	410	GLN
3	C	472	CYS
3	C	511	GLN
3	C	536	LEU
3	C	540	PRO
4	D	619	ASN
4	D	636	PRO
4	D	639	GLN
4	D	657	SER
4	D	679	HIS
4	D	705	PRO
4	D	775	TYR
4	D	778	VAL
4	D	847	ASP
5	E	886	ARG
5	E	907	ARG
5	E	932	SER
5	E	954	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	145	GLN
1	A	204	GLN
1	A	234	GLN
1	A	237	GLN
1	A	303	GLN
1	A	326	ASN

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Mol	Chain	Res	Type
2	B	410	GLN
3	C	445	HIS
3	C	511	GLN
4	D	628	ASN
4	D	639	GLN
4	D	667	ASN
4	D	699	GLN
4	D	707	GLN
4	D	748	ASN
4	D	779	ASN
4	D	790	GLN
4	D	814	HIS
5	E	888	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 ⓘ

15 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	$\# Z  > 2$
10	NDG	C	1	10,3	14,14,15	0.60	0	15,19,21	0.97	0
10	MAN	C	13	10	11,11,12	0.85	1 (9%)	14,15,17	0.95	0
10	MAN	C	14	10	11,11,12	1.61	2 (18%)	14,15,17	3.18	4 (28%)
10	MAN	C	16	10	11,11,12	0.45	0	14,15,17	0.95	1 (7%)
10	MAN	C	163	10	11,11,12	0.54	0	14,15,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	C	166	10	11,11,12	0.51	0	14,15,17	0.77	1 (7%)
10	MAN	C	167	10	11,11,12	0.39	0	14,15,17	0.78	1 (7%)
10	NAG	C	2	10	14,14,15	0.56	0	15,19,21	0.93	1 (6%)
10	BMA	C	3	10	11,11,12	0.43	0	14,15,17	0.63	0
11	NAG	D	1	11,4	14,14,15	0.76	0	15,19,21	0.89	0
11	NDG	D	11	11	14,14,15	0.82	0	15,19,21	1.04	1 (6%)
12	NAG	D	2	12,4	14,14,15	0.55	0	15,19,21	0.95	1 (6%)
12	NAG	D	21	12	14,14,15	0.58	0	15,19,21	0.76	0
12	NAG	D	3	12,4	14,14,15	0.74	0	15,19,21	1.06	1 (6%)
12	NAG	D	31	12	14,14,15	0.61	0	15,19,21	0.93	1 (6%)

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
10	NDG	C	1	10,3	-	0/6/23/26	0/1/1/1
10	MAN	C	13	10	-	0/2/19/22	0/1/1/1
10	MAN	C	14	10	-	0/2/19/22	0/1/1/1
10	MAN	C	16	10	-	0/2/19/22	0/1/1/1
10	MAN	C	163	10	-	0/2/19/22	0/1/1/1
10	MAN	C	166	10	-	0/2/19/22	0/1/1/1
10	MAN	C	167	10	-	0/2/19/22	0/1/1/1
10	NAG	C	2	10	-	0/6/23/26	0/1/1/1
10	BMA	C	3	10	-	0/2/19/22	0/1/1/1
11	NAG	D	1	11,4	-	0/6/23/26	0/1/1/1
11	NDG	D	11	11	-	0/6/23/26	0/1/1/1
12	NAG	D	2	12,4	-	0/6/23/26	0/1/1/1
12	NAG	D	21	12	-	0/6/23/26	0/1/1/1
12	NAG	D	3	12,4	-	0/6/23/26	0/1/1/1
12	NAG	D	31	12	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	14	MAN	C1-C2	-3.13	1.44	1.52
10	C	13	MAN	C2-C3	2.42	1.55	1.52
10	C	14	MAN	O5-C1	2.97	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	14	MAN	O3-C3-C2	-4.14	102.52	110.00
10	C	2	NAG	C2-N2-C7	-3.09	119.06	123.04
11	D	11	NDG	C2-N2-C7	-2.83	119.41	123.04
12	D	31	NAG	C2-N2-C7	-2.56	119.75	123.04
12	D	3	NAG	C2-N2-C7	-2.45	119.89	123.04
12	D	2	NAG	C2-N2-C7	-2.45	119.89	123.04
10	C	166	MAN	C1-O5-C5	2.05	114.85	112.25
10	C	167	MAN	C1-O5-C5	2.16	114.99	112.25
10	C	16	MAN	C1-O5-C5	2.64	115.60	112.25
10	C	14	MAN	C1-O5-C5	3.99	117.31	112.25
10	C	14	MAN	C6-C5-C4	6.24	128.42	113.02
10	C	14	MAN	C1-C2-C3	7.48	118.39	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1	NDG	5	0
10	C	2	NAG	4	0
11	D	1	NAG	3	0
11	D	11	NDG	3	0
12	D	2	NAG	4	0
12	D	21	NAG	2	0
12	D	3	NAG	1	0
12	D	31	NAG	1	0

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
6	NAG	A	1	1	14,14,15	0.71	0	15,19,21	0.89	1 (6%)
7	TRS	A	2	8	7,7,7	2.88	3 (42%)	9,9,9	1.43	2 (22%)
9	SO4	A	3001	-	4,4,4	0.79	0	6,6,6	0.23	0
9	SO4	E	3002	-	4,4,4	0.87	0	6,6,6	0.21	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
6	NAG	A	1	1	-	2/6/23/26	0/1/1/1
7	TRS	A	2	8	-	0/9/9/9	0/0/0/0
9	SO4	A	3001	-	-	0/0/0/0	0/0/0/0
9	SO4	E	3002	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2	TRS	C-N	-5.51	1.42	1.50
7	A	2	TRS	C3-C	3.23	1.59	1.53
7	A	2	TRS	C2-C	3.64	1.60	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2	TRS	C2-C-N	-2.34	103.83	108.09
6	A	1	NAG	C2-N2-C7	-2.19	120.22	123.04
7	A	2	TRS	C2-C-C1	2.12	115.38	110.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1	NAG	C8-C7-N2-C2
6	A	1	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1	NAG	1	0
7	A	2	TRS	1	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	292/298 (97%)	-0.55	0 <b>100</b> <b>100</b>	22, 36, 54, 76	0
2	B	76/84 (90%)	-0.48	1 (1%) <b>79</b> <b>79</b>	18, 35, 70, 87	0
3	C	151/159 (94%)	-0.64	0 <b>100</b> <b>100</b>	22, 36, 56, 95	0
4	D	270/282 (95%)	-0.51	1 (0%) <b>93</b> <b>94</b>	21, 38, 58, 94	0
5	E	109/126 (86%)	-0.63	0 <b>100</b> <b>100</b>	16, 38, 59, 92	0
All	All	898/949 (94%)	-0.56	2 (0%) <b>95</b> <b>96</b>	16, 37, 58, 95	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	ALA	3.6
4	D	875	GLY	2.4

### 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 [i](#)

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
11	NAG	D	1	14/15	0.93	0.18	0.68	50,50,50,50	0
10	NDG	C	1	14/15	0.95	0.12	0.20	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MAN	C	167	11/12	0.96	0.10	-0.33	27,27,27,27	0
10	NAG	C	2	14/15	0.96	0.10	-0.39	25,25,25,25	0
12	NAG	D	2	14/15	0.92	0.10	-1.56	46,46,46,46	0
10	MAN	C	166	11/12	0.92	0.14	-	32,32,32,32	0
10	MAN	C	13	11/12	0.95	0.15	-	44,44,44,44	0
10	MAN	C	14	11/12	0.83	0.18	-	72,72,72,72	0
10	MAN	C	163	11/12	0.89	0.20	-	57,57,57,57	0
11	NDG	D	11	14/15	0.86	0.32	-	79,79,79,79	0
10	MAN	C	16	11/12	0.94	0.11	-	33,33,33,33	0
10	BMA	C	3	11/12	0.97	0.10	-	33,33,33,33	0
12	NAG	D	3	14/15	0.94	0.20	-	44,44,44,44	0
12	NAG	D	21	14/15	0.90	0.22	-	67,67,67,67	0
12	NAG	D	31	14/15	0.91	0.29	-	75,75,75,75	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( $\text{\AA}^2$ )	Q<0.9
7	TRS	A	2	8/8	0.88	0.23	2.99	35,35,35,35	0
8	ZN	A	3	1/1	0.99	0.10	-1.56	35,35,35,35	0
9	SO4	A	3001	5/5	0.97	0.20	-	36,36,36,36	0
6	NAG	A	1	14/15	0.84	0.32	-	57,57,57,57	0
9	SO4	E	3002	5/5	0.98	0.14	-	36,36,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.