



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 04:47 AM GMT

PDB ID : 1O7D
Title : THE STRUCTURE OF THE BOVINE LYSOSOMAL A-MANNOSIDASE
SUGGESTS A NOVEL MECHANISM FOR LOW PH ACTIVATION
Authors : Heikinheimo, P.; Helland, R.; Leiros, H.S.; Leiros, I.; Karlsen, S.; Evjen,
G.; Ravelli, R.; Schoehn, G.; Ruigrok, R.; Tollersrud, O.-K.; Mcsweeney, S.;
Hough, E.
Deposited on : 2002-10-30
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

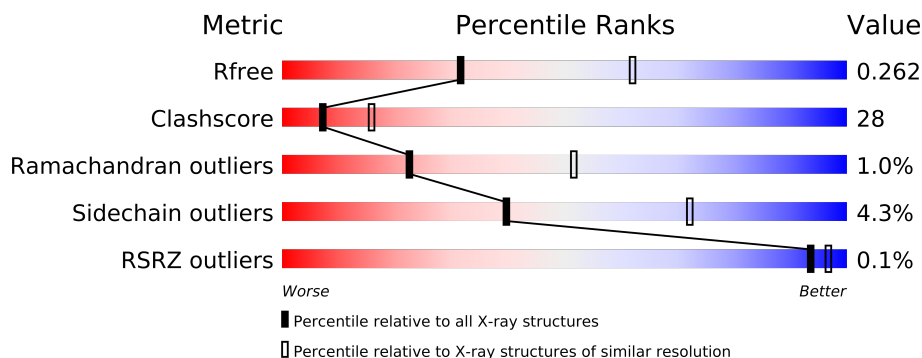
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	298	
2	B	84	
3	C	159	
4	D	282	
5	E	126	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	TRS	A	2	-	X
9	SO4	A	3001	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7385 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

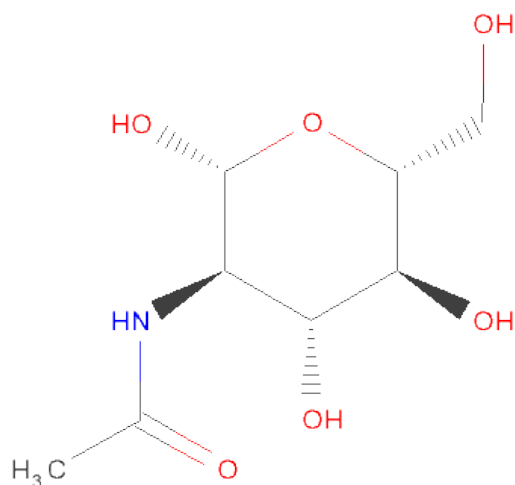
- Molecule 4 is a protein called LYSOSOMAL ALPHA-MANNOSIDASE.

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.

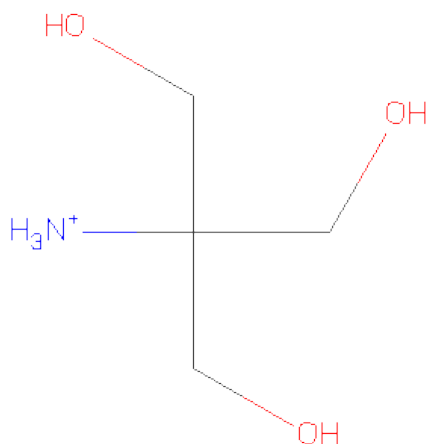
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	109	Total	C	N	O	S	0	0	1
			851	543	148	159	1			

- 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: $C_4H_{12}NO_3$).

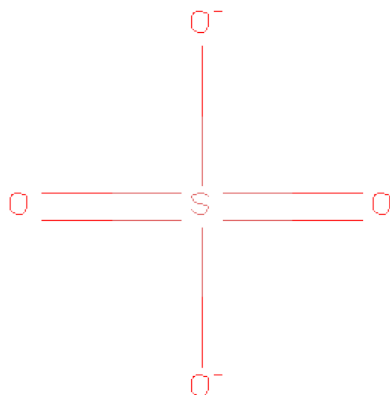


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		

- 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: O₄S).



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.

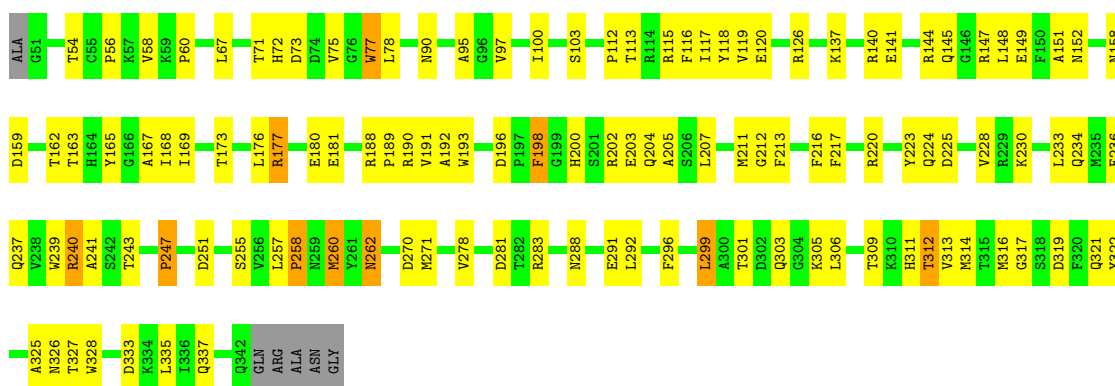
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	14	Total	O	0	0
			14	14		
13	B	2	Total	O	0	0
			2	2		
13	C	3	Total	O	0	0
			3	3		
13	D	14	Total	O	0	0
			14	14		
13	E	6	Total	O	0	0
			6	6		

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.

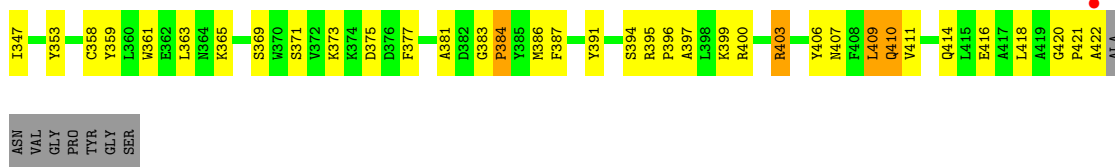
• Molecule 1: LYSOSOMAL ALPHA-MANNOSIDASE

Chain A: 



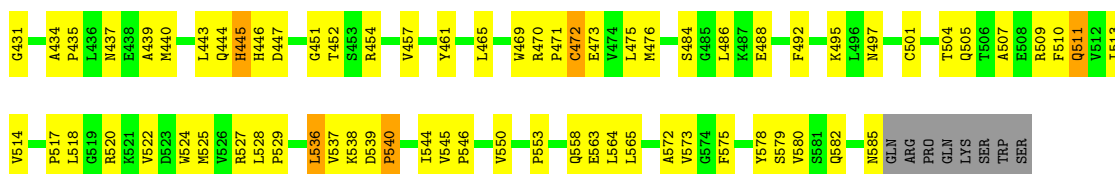
• Molecule 2: LYSOSOMAL ALPHA-MANNOSIDASE

Chain B: 



• Molecule 3: LYSOSOMAL ALPHA-MANNOSIDASE

Chain C: 



• Molecule 4: LYSOSOMAL ALPHA-MANNOSIDASE

Chain D: 



THR	P885
PRO	R886
HIS	T887
PRO	U888
SER	F889
PRO	S890
SER	S899
ARG	PRO
VAL	R901
SER	L905
A988	A906
T989	R907
P994	V908
M995	T912
F996	L913
I997	R916
R998	L917
T999	E918
A1002	R919
W1006	Q920
E1007	F921
GLU	A922
ASP	E925
GLY	D926
	S927
	G928
	R929
	N930
	L931
	S932
	T936
	L937
	D938
	L939
	T940
	N941
	F946
	L961
	R962
	E963
	T964
	T965
	L966
	A967
	A968
	R967
	D973
	T978
	GLY
	PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	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) 85.9 (29.62-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.289 0.266 , 0.262	Depositor DCC
R_{free} test set	3584 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 18.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2365	0	2290	129	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	622	0	587	48	0
3	C	1136	0	1106	91	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (409) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:240:ARG:HG2	1:A:251:ASP:OD1	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

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%)	22	51
2	B	74/84 (88%)	68 (92%)	5 (7%)	1 (1%)	16	41
3	C	149/159 (94%)	133 (89%)	15 (10%)	1 (1%)	30	62
4	D	266/282 (94%)	247 (93%)	16 (6%)	3 (1%)	21	49
5	E	105/126 (83%)	98 (93%)	6 (6%)	1 (1%)	22	51
All	All	884/949 (93%)	808 (91%)	67 (8%)	9 (1%)	22	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	920	GLN
1	A	77	TRP
2	B	421	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	42	75
2	B	65/71 (92%)	59 (91%)	6 (9%)	13	29
3	C	125/139 (90%)	121 (97%)	4 (3%)	51	82
4	D	227/240 (95%)	218 (96%)	9 (4%)	42	75
5	E	93/111 (84%)	89 (96%)	4 (4%)	40	72
All	All	761/821 (93%)	728 (96%)	33 (4%)	40	72

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 chains 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	12,14,15	0.45	0	15,19,21	0.96	0
10	MAN	C	13	10	10,11,12	0.65	0	11,15,17	0.86	1 (9%)
10	MAN	C	14	10	10,11,12	0.96	0	11,15,17	2.56	3 (27%)
10	MAN	C	16	10	10,11,12	0.45	0	11,15,17	0.50	0
10	MAN	C	163	10	10,11,12	0.50	0	11,15,17	0.60	0
10	MAN	C	166	10	10,11,12	0.46	0	11,15,17	0.44	0
10	MAN	C	167	10	10,11,12	0.40	0	11,15,17	0.53	0
10	NAG	C	2	10	12,14,15	0.69	0	15,19,21	0.91	1 (6%)
10	BMA	C	3	10	10,11,12	0.54	0	11,15,17	0.68	0
11	NAG	D	1	11,4	12,14,15	0.78	0	15,19,21	1.07	1 (6%)
11	NDG	D	11	11	12,14,15	0.71	0	15,19,21	0.92	1 (6%)
12	NAG	D	2	12,4	12,14,15	0.64	0	15,19,21	0.88	0
12	NAG	D	21	12	12,14,15	0.54	0	15,19,21	0.66	0
12	NAG	D	3	12,4	12,14,15	0.69	0	15,19,21	0.97	0
12	NAG	D	31	12	12,14,15	0.49	0	15,19,21	0.93	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
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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	14	MAN	C6-C5-C4	6.38	128.42	113.00
10	C	14	MAN	O3-C3-C2	-4.05	102.52	109.94
10	C	2	NAG	C2-N2-C7	-2.40	119.06	123.09
11	D	1	NAG	C3-C2-N2	-2.27	108.30	111.76
10	C	14	MAN	C4-C3-C2	2.19	113.45	110.50
11	D	11	NDG	C2-N2-C7	-2.19	119.41	123.09
10	C	13	MAN	C4-C3-C2	2.12	113.35	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	12,14,15	0.63	0	15,19,21	0.89	0
7	TRS	A	2	8	7,7,7	2.81	3 (42%)	9,9,9	1.48	1 (11%)
9	SO4	A	3001	-	4,4,4	0.86	0	6,6,6	0.23	0
9	SO4	E	3002	-	4,4,4	0.94	0	6,6,6	0.19	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	-5.62	1.42	1.50
7	A	2	TRS	C2-C	3.29	1.60	1.53
7	A	2	TRS	C3-C	2.92	1.59	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2	TRS	C2-C-C1	2.85	115.38	110.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	292/298 (97%)	-0.54	0 100 100	22, 36, 54, 76	0
2	B	76/84 (90%)	-0.45	1 (1%) 74 79	18, 35, 70, 87	0
3	C	151/159 (94%)	-0.61	0 100 100	22, 36, 56, 95	0
4	D	270/282 (95%)	-0.50	0 100 100	21, 38, 58, 94	0
5	E	109/126 (86%)	-0.61	0 100 100	16, 38, 59, 92	0
All	All	898/949 (94%)	-0.54	1 (0%) 93 97	16, 37, 58, 95	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	ALA	4.2

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	NAG	D	31	14/15	0.26	9.09	75,75,75,75	0
10	MAN	C	14	11/12	0.19	5.06	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	MAN	C	166	11/12	0.13	4.38	32,32,32,32	0
12	NAG	D	3	14/15	0.18	3.00	44,44,44,44	0
10	MAN	C	13	11/12	0.16	2.77	44,44,44,44	0
12	NAG	D	21	14/15	0.22	1.69	67,67,67,67	0
11	NAG	D	1	14/15	0.17	0.77	50,50,50,50	0
10	MAN	C	16	11/12	0.10	0.44	33,33,33,33	0
10	NDG	C	1	14/15	0.12	0.11	31,31,31,31	0
10	BMA	C	3	11/12	0.10	-0.19	33,33,33,33	0
10	MAN	C	167	11/12	0.10	-0.61	27,27,27,27	0
10	NAG	C	2	14/15	0.10	-0.71	25,25,25,25	0
12	NAG	D	2	14/15	0.10	-1.15	46,46,46,46	0
10	MAN	C	163	11/12	0.19	-1.80	57,57,57,57	0
11	NDG	D	11	14/15	0.33	-	79,79,79,79	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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	SO4	A	3001	5/5	0.19	9.35	36,36,36,36	0
7	TRS	A	2	8/8	0.22	2.85	35,35,35,35	0
9	SO4	E	3002	5/5	0.11	-0.60	36,36,36,36	0
8	ZN	A	3	1/1	0.11	-1.80	35,35,35,35	0
6	NAG	A	1	14/15	0.32	-	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.