



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2017 – 12:19 AM EDT

PDB ID : 1N1M
Title : Human Dipeptidyl Peptidase IV/CD26 in complex with an inhibitor
Authors : Rasmussen, H.B.; Branner, S.; Wiberg, F.C.; Wagtmann, N.R.
Deposited on : unknown
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

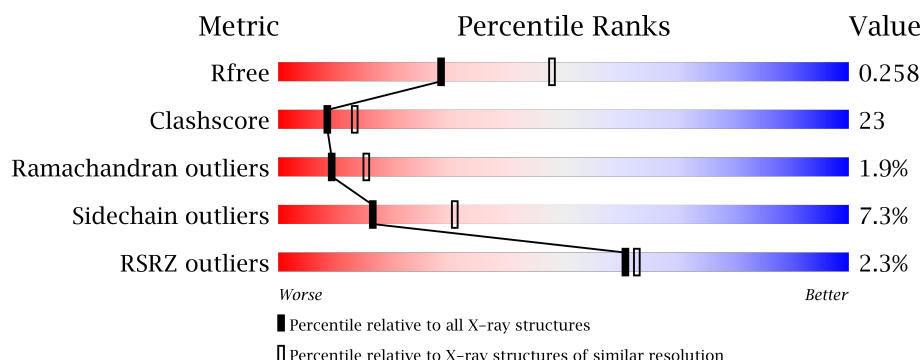
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>32%</div> <div>5%</div> </div> </div>
1	B	728	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>35%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	767	-	-	-	X
2	NAG	A	774	-	-	-	X
2	NAG	A	782	-	-	X	-
2	NAG	B	771	-	-	-	X
2	NAG	B	780	-	-	-	X
3	NDG	A	776	-	-	X	-
3	NDG	B	778	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13270 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 Dipeptidyl peptidase IV SOLUBLE FORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



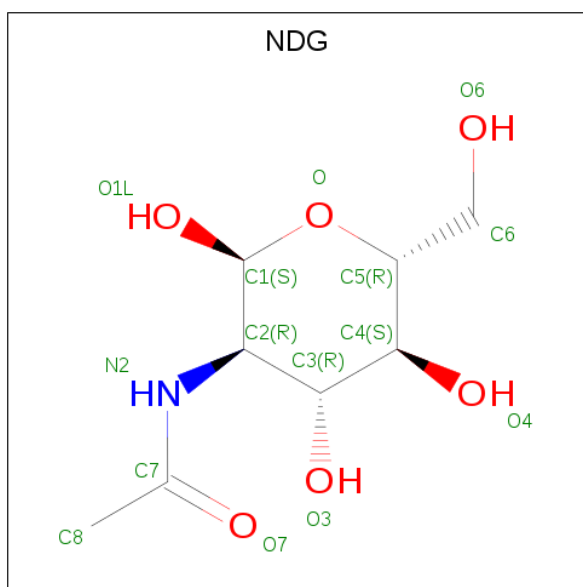
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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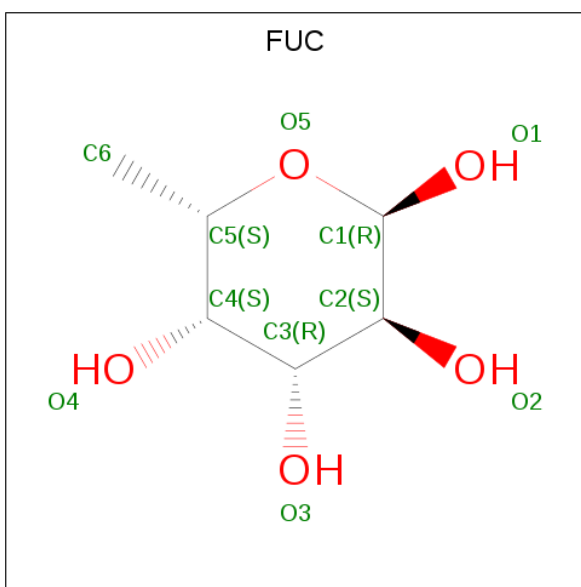
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

- Molecule 3 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: C₈H₁₅NO₆).



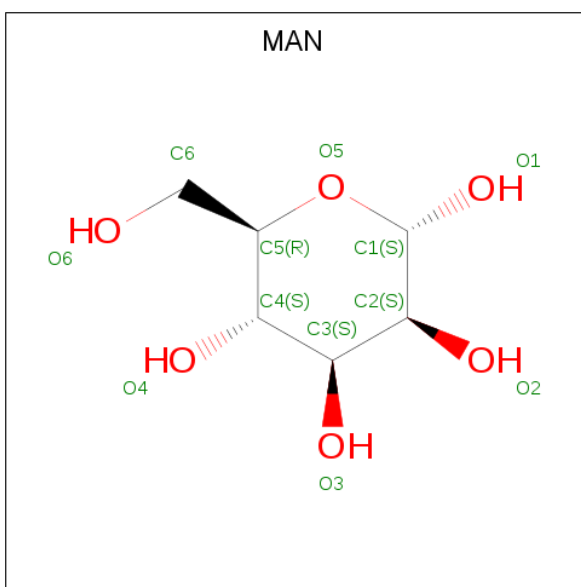
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

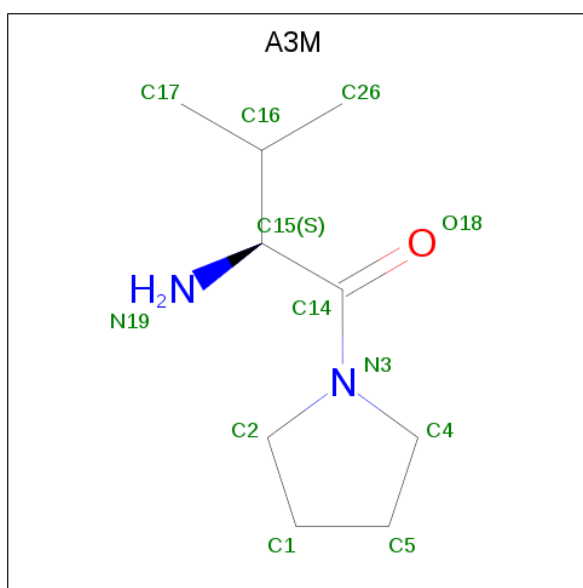


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

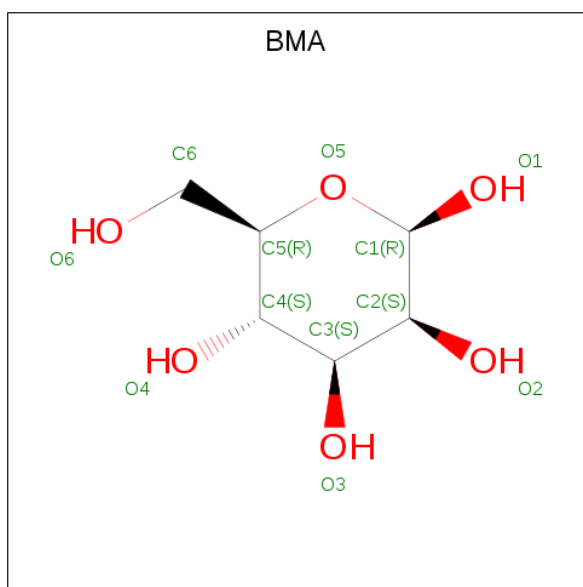
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Hg	0	0
			2	2		
6	A	2	Total	Hg	0	0
			2	2		

- Molecule 7 is 2-AMINO-3-METHYL-1-PYRROLIDIN-1-YL-BUTAN-1-ONE (three-letter code: A3M) (formula: C₉H₁₈N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			12	9	2	1		
7	B	1	Total	C	N	O	0	0
			12	9	2	1		

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		

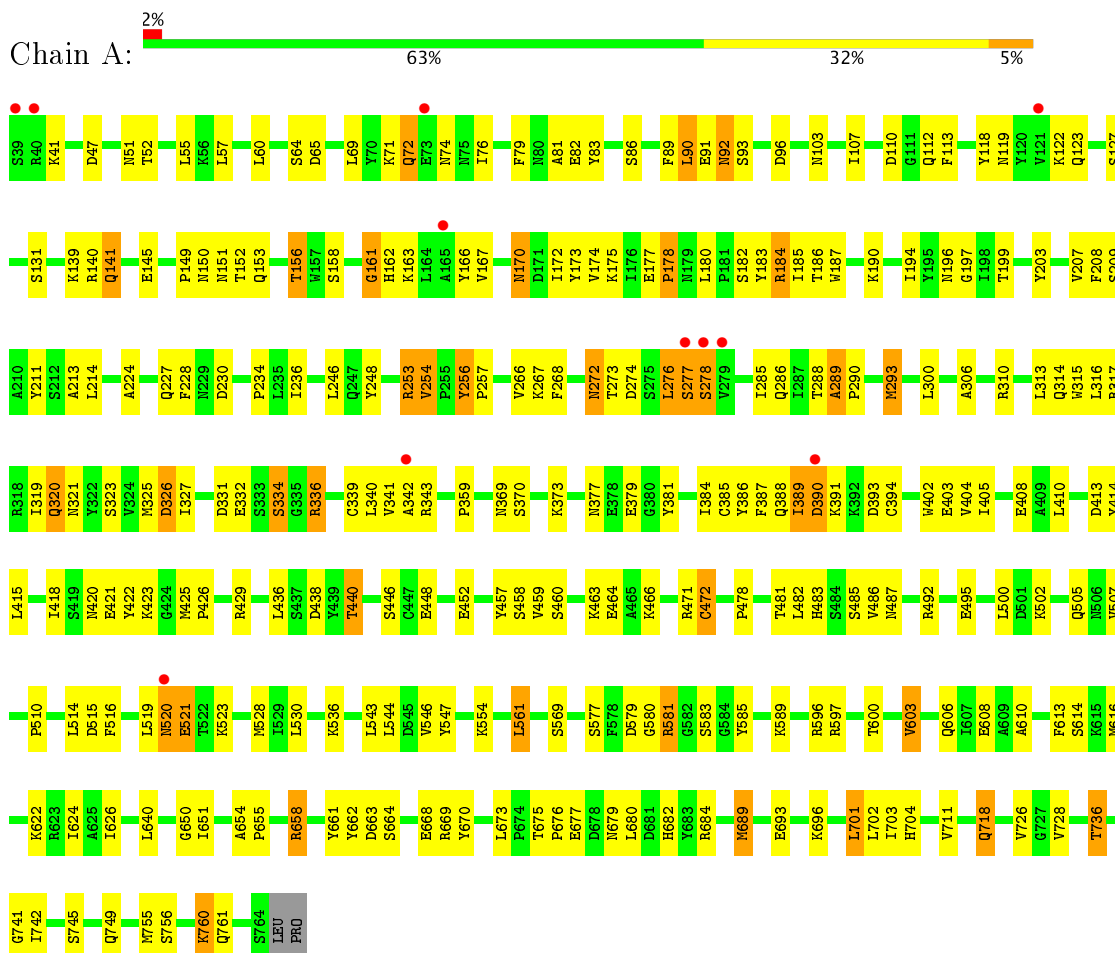
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	488	Total	O	0	0
			488	488		
9	B	443	Total	O	0	0
			443	443		

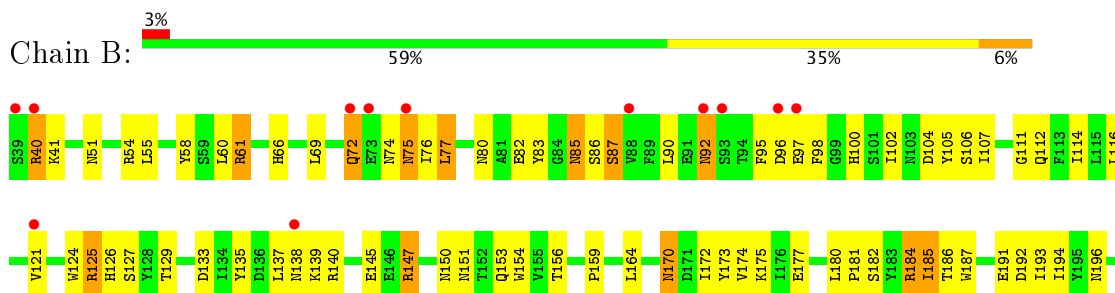
3 Residue-property plots

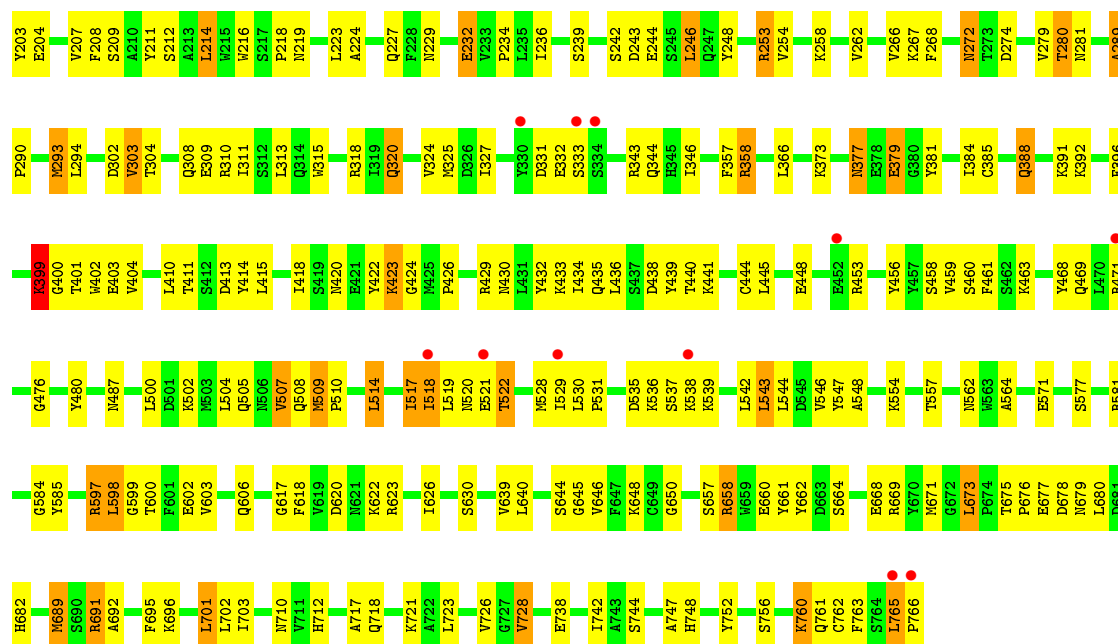
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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: Dipeptidyl peptidase IV SOLUBLE FORM



● Molecule 1: Dipeptidyl peptidase IV SOLUBLE FORM





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.23Å 123.45Å 131.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.50 29.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.2 (29.98-2.50) 87.3 (29.98-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.51Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.208 , 0.263 0.205 , 0.258	Depositor DCC
R_{free} test set	2987 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13270	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG, FUC, HG, A3M, 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	0.35	0/6119	0.65	0/8321
1	B	0.34	0/6136	0.65	1/8344 (0.0%)
All	All	0.35	0/12255	0.65	1/16665 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	LYS	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5948	0	5657	247	0
1	B	5964	0	5673	282	0
2	A	140	0	124	25	0
2	B	112	0	99	6	0
3	A	42	0	36	17	0
3	B	42	0	37	8	0
4	A	20	0	20	2	0
4	B	10	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	11	0	10	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	12	0	18	2	0
7	B	12	0	18	3	0
8	B	22	0	20	1	0
9	A	488	0	0	15	0
9	B	443	0	0	29	0
All	All	13270	0	11722	552	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 23.

All (552) 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:A:776:NDG:H6C2	5:A:777:MAN:H2	1.26	1.13
1:A:581:ARG:CZ	2:A:782:NAG:H61	1.81	1.08
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.33	1.06
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.40	1.02
1:B:172:ILE:HG22	1:B:185:ILE:HD11	1.42	1.00
3:B:778:NDG:H6C2	3:B:779:NDG:HA	1.25	0.98
1:B:203:TYR:CD2	1:B:207:VAL:HG21	2.01	0.95
1:B:61:ARG:HH22	1:B:107:ILE:H	1.17	0.93
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.31	0.93
1:B:72:GLN:HE21	1:B:77:LEU:HD21	1.30	0.92
1:B:308:GLN:HG3	3:B:770:NDG:H6C2	1.49	0.92
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.00	0.91
3:B:778:NDG:H6C2	3:B:779:NDG:N2	1.83	0.91
1:A:172:ILE:H	1:A:186:THR:HG22	1.35	0.91
1:A:110:ASP:HB3	1:A:112:GLN:HG3	1.53	0.90
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.53	0.90
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.69	0.90
1:A:253:ARG:HH22	1:B:253:ARG:NH2	1.69	0.89
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.04	0.88
1:A:172:ILE:H	1:A:186:THR:CG2	1.86	0.88
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.73	0.88
3:A:770:NDG:H4	2:A:771:NAG:HN2	1.36	0.88
1:A:276:LEU:H	1:A:276:LEU:HD23	1.39	0.87
3:B:778:NDG:O3	3:B:779:NDG:H5	1.75	0.87
1:B:358:ARG:HH11	1:B:358:ARG:HB3	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:756:SER:O	1:B:760:LYS:HG2	1.75	0.86
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.58	0.85
1:B:175:LYS:HG2	1:B:182:SER:HB3	1.59	0.84
1:B:318:ARG:HD3	1:B:668:GLU:OE1	1.77	0.84
1:B:40:ARG:NH1	1:B:508:GLN:HG2	1.92	0.83
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.76	0.83
1:B:72:GLN:NE2	1:B:77:LEU:HD21	1.92	0.83
1:B:399:LYS:HB2	1:B:402:TRP:HZ2	1.45	0.81
1:B:399:LYS:HB2	1:B:402:TRP:CZ2	2.15	0.81
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.15	0.81
1:B:676:PRO:HG2	1:B:677:GLU:OE2	1.81	0.80
1:A:194:ILE:HD13	2:A:775:NAG:H82	1.62	0.80
2:A:782:NAG:H4	9:A:1109:HOH:O	1.82	0.80
3:A:776:NDG:H6C2	5:A:777:MAN:C2	2.11	0.78
1:B:528:MET:HE2	1:B:530:LEU:HD21	1.63	0.78
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.82	0.78
1:A:736:THR:HG21	1:B:717:ALA:O	1.83	0.78
3:A:770:NDG:H4	2:A:771:NAG:N2	1.96	0.78
1:A:600:THR:O	1:A:603:VAL:HG13	1.85	0.77
1:A:289:ALA:HB2	9:A:1181:HOH:O	1.85	0.77
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.67	0.76
1:B:77:LEU:H	1:B:77:LEU:HD23	1.48	0.76
1:B:377:ASN:HD22	1:B:377:ASN:C	1.88	0.76
1:B:184:ARG:HD3	1:B:186:THR:O	1.87	0.75
1:B:504:LEU:HD22	1:B:509:MET:HE2	1.68	0.74
1:A:253:ARG:HH22	1:B:253:ARG:HH22	0.85	0.74
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.68	0.74
1:B:60:LEU:HD13	1:B:469:GLN:OE1	1.87	0.73
1:B:121:VAL:HB	1:B:129:THR:CG2	2.19	0.73
1:B:644:SER:O	1:B:646:VAL:N	2.22	0.73
1:B:691:ARG:HD2	9:B:1156:HOH:O	1.88	0.73
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.70	0.72
1:A:613:PHE:O	1:A:616:MET:HB2	1.89	0.72
1:A:74:ASN:HB3	1:A:92:ASN:OD1	1.89	0.72
1:B:90:LEU:HD21	1:B:95:PHE:CE2	2.21	0.72
1:A:452:GLU:HG3	9:A:1410:HOH:O	1.88	0.72
1:B:112:GLN:HB3	1:B:138:ASN:HD21	1.55	0.72
1:A:203:TYR:HA	1:A:207:VAL:CG1	2.20	0.72
1:B:207:VAL:HG23	1:B:208:PHE:N	2.05	0.71
1:A:438:ASP:OD1	1:A:440:THR:HB	1.90	0.71
1:B:377:ASN:ND2	1:B:379:GLU:H	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ASP:HB3	1:A:583:SER:OG	1.90	0.71
1:A:203:TYR:HA	1:A:207:VAL:HG12	1.72	0.71
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.25	0.71
1:A:414:TYR:HA	1:A:436:LEU:HD13	1.71	0.71
1:B:308:GLN:OE1	1:B:308:GLN:HA	1.91	0.71
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.06	0.70
1:B:219:ASN:HB2	1:B:308:GLN:CD	2.12	0.70
1:B:504:LEU:HD22	1:B:509:MET:CE	2.20	0.70
1:B:308:GLN:CG	3:B:770:NDG:H6C2	2.22	0.70
1:B:509:MET:HG3	1:B:510:PRO:HD2	1.74	0.69
1:B:327:ILE:HB	1:B:343:ARG:HG2	1.74	0.69
1:B:232:GLU:HB3	1:B:262:VAL:HG11	1.75	0.69
1:B:517:ILE:HG12	1:B:518:ILE:N	2.08	0.69
1:A:319:ILE:HG22	1:A:321:ASN:HB2	1.75	0.69
2:A:767:NAG:O3	3:A:768:NDG:H5	1.92	0.68
1:B:520:ASN:O	1:B:522:THR:HG22	1.94	0.68
1:B:77:LEU:N	1:B:77:LEU:HD23	2.09	0.68
1:B:170:ASN:N	1:B:170:ASN:HD22	1.91	0.68
1:A:82:GLU:HG2	9:A:1241:HOH:O	1.93	0.68
3:A:776:NDG:C6	5:A:777:MAN:H2	2.14	0.68
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.94	0.68
1:A:272:ASN:ND2	1:A:274:ASP:H	1.92	0.67
1:B:76:ILE:CG2	1:B:90:LEU:HB3	2.25	0.67
1:B:279:VAL:O	1:B:280:THR:HB	1.92	0.67
1:B:51:ASN:HD21	1:B:54:ARG:HD3	1.57	0.67
1:A:290:PRO:HG3	1:A:326:ASP:OD2	1.94	0.67
1:B:546:VAL:HG22	1:B:547:TYR:N	2.10	0.67
1:A:276:LEU:N	1:A:276:LEU:HD23	2.11	0.66
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.31	0.66
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.77	0.66
1:A:340:LEU:O	1:A:343:ARG:HB3	1.97	0.65
1:B:74:ASN:O	1:B:92:ASN:HA	1.95	0.65
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.31	0.65
1:A:289:ALA:CB	1:A:290:PRO:CA	2.75	0.65
1:B:74:ASN:HB3	1:B:92:ASN:OD1	1.97	0.65
1:B:522:THR:HG21	9:B:1153:HOH:O	1.94	0.65
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.95	0.65
1:B:121:VAL:HA	9:B:1250:HOH:O	1.96	0.65
1:A:194:ILE:CD1	2:A:775:NAG:H82	2.27	0.65
1:B:765:LEU:HB3	1:B:766:PRO:OXT	1.98	0.64
1:A:289:ALA:CB	1:A:290:PRO:HA	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.79	0.64
1:A:76:ILE:HD12	1:A:90:LEU:HD11	1.79	0.64
1:B:54:ARG:HD3	9:B:1321:HOH:O	1.98	0.64
2:A:771:NAG:C3	2:A:771:NAG:O7	2.45	0.64
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.97	0.63
1:B:302:ASP:OD1	1:B:304:THR:HG23	1.98	0.63
1:B:402:TRP:HA	9:B:1148:HOH:O	1.98	0.63
1:B:502:LYS:O	1:B:505:GLN:HG2	1.98	0.63
1:B:86:SER:O	1:B:87:SER:HB2	1.98	0.63
2:A:771:NAG:H3	2:A:771:NAG:O7	1.97	0.63
3:A:776:NDG:H3	3:A:776:NDG:O7	1.97	0.63
1:A:520:ASN:O	1:A:521:GLU:HB2	1.97	0.63
1:B:112:GLN:HB3	1:B:138:ASN:ND2	2.13	0.63
1:B:723:LEU:HB3	1:B:728:VAL:HG13	1.79	0.63
1:A:203:TYR:CD2	1:A:207:VAL:HG11	2.34	0.62
1:A:47:ASP:HA	1:A:52:THR:HG23	1.80	0.62
1:B:279:VAL:HG23	1:B:280:THR:H	1.64	0.62
1:B:280:THR:HG23	1:B:281:ASN:N	2.13	0.62
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.35	0.62
1:B:289:ALA:CB	1:B:290:PRO:HA	2.22	0.62
1:B:61:ARG:NH2	1:B:107:ILE:H	1.95	0.62
1:A:76:ILE:HB	1:A:90:LEU:CD1	2.29	0.62
1:A:377:ASN:HB2	1:A:381:TYR:H	1.65	0.62
1:A:756:SER:O	1:A:760:LYS:HG2	2.00	0.61
1:B:125:ARG:HG2	1:B:126:HIS:CE1	2.35	0.61
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.63	0.61
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.97	0.61
1:A:662:TYR:CE2	7:A:954:A3M:HC21	2.36	0.61
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.00	0.61
2:A:782:NAG:H62	9:A:1179:HOH:O	2.01	0.61
1:B:75:ASN:ND2	1:B:92:ASN:HB2	2.14	0.60
1:A:341:VAL:O	1:A:342:ALA:HB3	2.01	0.60
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.35	0.60
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.46	0.60
1:A:341:VAL:C	1:A:343:ARG:H	2.04	0.60
2:A:782:NAG:O7	2:A:782:NAG:H3	2.00	0.60
1:B:765:LEU:CB	1:B:766:PRO:HA	2.32	0.60
1:B:147:ARG:HG3	9:B:1255:HOH:O	2.01	0.60
1:B:554:LYS:HB3	1:B:577:SER:HB3	1.83	0.60
1:B:358:ARG:HD2	9:B:1229:HOH:O	2.01	0.59
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:SER:HB3	1:A:336:ARG:HD2	1.84	0.59
1:B:203:TYR:HA	1:B:207:VAL:HG22	1.84	0.59
1:A:272:ASN:C	1:A:272:ASN:HD22	2.05	0.59
1:A:651:ILE:HG21	1:A:755:MET:HE3	1.85	0.59
1:B:744:SER:HB3	1:B:747:ALA:HB3	1.84	0.59
1:B:571:GLU:OE1	1:B:765:LEU:HD22	2.02	0.59
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.68	0.58
1:B:279:VAL:O	1:B:280:THR:CB	2.50	0.58
1:A:172:ILE:N	1:A:186:THR:HG22	2.14	0.58
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.85	0.58
1:B:332:GLU:OE2	2:B:771:NAG:H4	2.03	0.58
1:A:502:LYS:O	1:A:505:GLN:HG2	2.02	0.58
1:B:207:VAL:CG2	1:B:208:PHE:N	2.66	0.58
1:B:344:GLN:HE21	1:B:346:ILE:HD11	1.68	0.58
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.34	0.58
1:B:83:TYR:CE2	4:B:768:FUC:H4	2.38	0.58
1:A:170:ASN:N	1:A:170:ASN:HD22	2.01	0.58
1:A:662:TYR:CZ	7:A:954:A3M:HC21	2.38	0.58
1:B:701:LEU:HD22	1:B:703:ILE:HG13	1.86	0.58
8:B:777:BMA:H4	9:B:1359:HOH:O	2.04	0.57
1:A:684:ARG:HG3	9:A:1149:HOH:O	2.04	0.57
1:B:648:LYS:HD3	1:B:762:CYS:SG	2.43	0.57
1:B:172:ILE:HG22	1:B:185:ILE:CD1	2.25	0.57
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.39	0.57
1:A:92:ASN:HD22	1:A:93:SER:H	1.51	0.57
1:B:150:ASN:O	1:B:151:ASN:HB2	2.04	0.57
3:B:778:NDG:H4	3:B:779:NDG:H3	1.85	0.57
1:A:187:TRP:HE3	2:A:779:NAG:H83	1.69	0.57
3:A:770:NDG:H6C2	4:A:772:FUC:O2	2.04	0.57
1:B:154:TRP:NE1	1:B:156:THR:HG23	2.19	0.57
1:B:203:TYR:O	1:B:207:VAL:HG22	2.05	0.57
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.69	0.57
1:B:373:LYS:HE2	9:B:1374:HOH:O	2.05	0.57
1:B:546:VAL:CG2	1:B:547:TYR:N	2.68	0.57
1:B:280:THR:CG2	1:B:281:ASN:N	2.68	0.56
1:A:581:ARG:NH2	2:A:782:NAG:H61	2.20	0.56
1:B:121:VAL:HB	1:B:129:THR:HG23	1.87	0.56
1:B:358:ARG:NH1	9:B:956:HOH:O	2.36	0.56
1:A:150:ASN:O	1:A:151:ASN:HB2	2.06	0.56
1:A:580:GLY:O	1:A:583:SER:HB2	2.06	0.56
1:B:194:ILE:HD13	1:B:229:ASN:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:MET:CE	1:A:530:LEU:HD21	2.35	0.56
1:A:236:ILE:HG22	1:A:254:VAL:O	2.06	0.56
1:A:272:ASN:HD22	1:A:274:ASP:H	1.54	0.56
1:B:121:VAL:HB	1:B:129:THR:HG22	1.87	0.56
1:B:177:GLU:HB2	1:B:180:LEU:HG	1.88	0.56
1:B:154:TRP:HE1	1:B:156:THR:CG2	2.18	0.56
1:B:377:ASN:ND2	1:B:379:GLU:N	2.54	0.56
1:B:58:TYR:HD1	1:B:60:LEU:HD11	1.71	0.56
1:A:149:PRO:HA	3:A:770:NDG:H8C3	1.86	0.56
1:B:529:ILE:HD13	9:B:1174:HOH:O	2.06	0.56
1:A:622:LYS:NZ	1:A:622:LYS:HB2	2.20	0.55
3:A:776:NDG:C3	3:A:776:NDG:O7	2.54	0.55
1:B:69:LEU:HD11	1:B:107:ILE:HD12	1.87	0.55
1:B:289:ALA:CB	1:B:290:PRO:CA	2.78	0.55
1:A:175:LYS:NZ	1:A:182:SER:HB2	2.20	0.55
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.88	0.55
1:B:606:GLN:NE2	9:B:964:HOH:O	2.39	0.55
1:A:341:VAL:HG22	1:A:342:ALA:H	1.72	0.55
1:A:369:ASN:O	1:A:389:ILE:HG23	2.05	0.55
1:B:518:ILE:HD11	1:B:521:GLU:HA	1.88	0.55
1:B:75:ASN:HD21	1:B:92:ASN:HB2	1.71	0.55
1:B:765:LEU:HB3	1:B:766:PRO:CA	2.36	0.55
1:A:156:THR:CG2	1:A:214:LEU:HD11	2.31	0.55
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.42	0.55
1:B:272:ASN:C	1:B:272:ASN:HD22	2.09	0.55
1:A:90:LEU:O	1:A:90:LEU:HD13	2.07	0.55
1:A:327:ILE:HB	1:A:343:ARG:HG2	1.89	0.55
1:A:92:ASN:ND2	1:A:92:ASN:H	2.02	0.55
1:B:86:SER:O	1:B:87:SER:CB	2.56	0.54
1:A:103:ASN:HB3	9:A:1436:HOH:O	2.07	0.54
1:A:174:VAL:HG23	1:A:185:ILE:HG13	1.89	0.54
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.43	0.54
1:B:765:LEU:CB	1:B:766:PRO:CA	2.85	0.54
1:B:164:LEU:HB2	1:B:175:LYS:HB2	1.89	0.54
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.06	0.54
1:B:358:ARG:HH11	1:B:358:ARG:CB	2.15	0.54
1:B:539:LYS:HE3	1:B:617:GLY:O	2.07	0.54
1:A:306:ALA:HB3	1:A:310:ARG:HB3	1.89	0.54
1:A:626:ILE:O	1:A:650:GLY:HA2	2.08	0.54
1:B:413:ASP:HB3	1:B:414:TYR:HD1	1.72	0.53
1:B:487:ASN:HB2	9:B:1324:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TRP:O	1:A:323:SER:HB2	2.08	0.53
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.43	0.53
1:B:147:ARG:HB3	1:B:147:ARG:HH11	1.74	0.53
1:A:65:ASP:HB2	1:A:464:GLU:HG2	1.90	0.53
1:B:765:LEU:HB2	1:B:766:PRO:HA	1.90	0.53
1:A:122:LYS:HG2	1:A:123:GLN:N	2.23	0.53
1:B:542:LEU:HD23	1:B:542:LEU:C	2.29	0.53
1:A:207:VAL:HG22	1:A:208:PHE:CD1	2.44	0.53
1:A:519:LEU:O	1:A:520:ASN:C	2.47	0.53
1:A:272:ASN:HD22	1:A:273:THR:N	2.06	0.53
1:A:651:ILE:HG21	1:A:755:MET:CE	2.38	0.53
1:A:597:ARG:HG3	1:A:600:THR:HG21	1.89	0.53
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.43	0.52
1:B:154:TRP:NE1	1:B:156:THR:CG2	2.72	0.52
1:A:93:SER:HA	1:A:96:ASP:OD1	2.10	0.52
1:B:598:LEU:HB2	1:B:671:MET:SD	2.49	0.52
1:A:377:ASN:HB2	1:A:381:TYR:N	2.23	0.52
1:B:415:LEU:HD23	1:B:415:LEU:C	2.29	0.52
1:A:388:GLN:O	1:A:390:ASP:N	2.42	0.52
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.45	0.52
1:B:318:ARG:HG2	9:B:988:HOH:O	2.10	0.52
1:B:519:LEU:O	1:B:522:THR:HG23	2.10	0.52
1:B:76:ILE:O	1:B:76:ILE:HG23	2.08	0.52
1:B:692:ALA:O	1:B:695:PHE:HB2	2.09	0.52
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	1.57	0.52
1:A:314:GLN:NE2	1:A:373:LYS:NZ	2.58	0.52
1:B:344:GLN:NE2	9:B:1038:HOH:O	2.42	0.52
1:B:418:ILE:HA	1:B:430:ASN:O	2.10	0.52
1:A:286:GLN:HE21	1:A:288:THR:HG22	1.75	0.52
1:A:589:LYS:HB3	9:A:964:HOH:O	2.09	0.52
1:A:405:ILE:HG13	1:A:429:ARG:CD	2.40	0.51
1:B:311:ILE:HG12	1:B:313:LEU:CD1	2.40	0.51
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.46	0.51
1:B:662:TYR:CE2	7:B:955:A3M:HC21	2.45	0.51
1:A:276:LEU:HD23	9:A:1345:HOH:O	2.09	0.51
1:B:377:ASN:C	1:B:377:ASN:ND2	2.61	0.51
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.92	0.51
1:A:158:SER:CB	1:A:163:LYS:HB2	2.40	0.51
1:A:334:SER:HB3	1:A:336:ARG:CD	2.40	0.51
1:B:236:ILE:HG22	1:B:254:VAL:O	2.09	0.51
1:B:98:PHE:CD1	1:B:100:HIS:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:HA	1:A:293:MET:HE2	1.92	0.51
1:A:546:VAL:CG2	1:A:547:TYR:N	2.74	0.51
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.93	0.51
1:B:536:LYS:HG2	1:B:618:PHE:CD2	2.46	0.51
1:B:344:GLN:O	1:B:392:LYS:HE2	2.11	0.50
1:B:95:PHE:O	1:B:98:PHE:HB2	2.11	0.50
1:A:610:ALA:HA	1:A:613:PHE:HD2	1.77	0.50
1:B:207:VAL:HG23	1:B:208:PHE:CD1	2.46	0.50
1:B:504:LEU:HD13	1:B:509:MET:HE2	1.92	0.50
1:A:745:SER:O	1:A:749:GLN:HG3	2.11	0.50
1:B:104:ASP:OD1	1:B:105:TYR:N	2.45	0.50
1:B:696:LYS:HD2	9:B:1382:HOH:O	2.11	0.50
1:B:181:PRO:HA	9:B:1378:HOH:O	2.12	0.50
1:B:207:VAL:CG2	1:B:208:PHE:H	2.25	0.50
1:B:289:ALA:HA	1:B:294:LEU:HG	1.94	0.50
1:A:293:MET:CE	1:A:317:ARG:HG3	2.42	0.50
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.94	0.50
1:B:520:ASN:HB2	2:B:780:NAG:H61	1.94	0.50
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.12	0.50
1:A:273:THR:O	1:A:276:LEU:HD21	2.11	0.49
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.12	0.49
1:B:518:ILE:HD13	1:B:518:ILE:C	2.32	0.49
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.47	0.49
1:A:314:GLN:HE22	1:A:373:LYS:NZ	2.10	0.49
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.27	0.49
1:B:280:THR:HB	9:B:1091:HOH:O	2.13	0.49
1:B:630:SER:OG	7:B:955:A3M:HC42	2.12	0.49
1:A:236:ILE:CG2	1:A:254:VAL:HG13	2.43	0.49
1:B:657:SER:HB2	1:B:689:MET:CE	2.43	0.49
1:A:664:SER:HB2	1:A:668:GLU:OE2	2.12	0.49
3:A:770:NDG:O6	2:A:771:NAG:H2	2.13	0.49
1:B:191:GLU:O	1:B:193:ILE:HG12	2.12	0.49
1:B:80:ASN:HB3	1:B:85:ASN:HB2	1.95	0.49
1:B:154:TRP:HE1	1:B:156:THR:HG23	1.77	0.49
1:B:385:CYS:HB3	1:B:396:PHE:CD1	2.47	0.49
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.94	0.49
1:B:696:LYS:HE3	9:B:1327:HOH:O	2.11	0.49
1:A:544:LEU:HD21	1:A:606:GLN:HG3	1.93	0.49
1:B:677:GLU:H	1:B:677:GLU:CD	2.16	0.49
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.45	0.49
1:B:738:GLU:OE2	1:B:744:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LYS:HD3	1:B:539:LYS:N	2.28	0.49
1:A:415:LEU:HB2	1:A:436:LEU:HD11	1.94	0.48
1:B:133:ASP:OD1	1:B:147:ARG:NH1	2.46	0.48
1:B:597:ARG:HG3	1:B:600:THR:HG21	1.94	0.48
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.48
1:B:581:ARG:CZ	2:B:780:NAG:H5	2.43	0.48
1:B:86:SER:O	2:B:767:NAG:H81	2.13	0.48
1:A:528:MET:HE2	1:A:530:LEU:HD21	1.96	0.48
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.79	0.48
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.49	0.48
1:B:325:MET:CE	1:B:373:LYS:HD2	2.44	0.48
1:B:58:TYR:CD1	1:B:60:LEU:HD11	2.48	0.48
1:B:174:VAL:HG23	1:B:185:ILE:HD12	1.94	0.48
1:B:599:GLY:N	1:B:602:GLU:OE2	2.31	0.48
1:A:736:THR:HG23	9:B:957:HOH:O	2.14	0.48
2:A:767:NAG:O3	3:A:768:NDG:C5	2.59	0.48
1:B:203:TYR:CA	1:B:207:VAL:HG22	2.44	0.48
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.96	0.48
1:B:60:LEU:HD13	1:B:469:GLN:CD	2.34	0.48
1:B:597:ARG:NH2	1:B:682:HIS:HB2	2.28	0.48
1:B:763:PHE:HB2	1:B:765:LEU:CD1	2.44	0.48
1:A:408:GLU:HG3	1:A:459:VAL:HG12	1.95	0.47
1:A:60:LEU:HD12	1:A:60:LEU:O	2.14	0.47
1:B:279:VAL:HG23	1:B:280:THR:N	2.28	0.47
1:B:453:ARG:HG3	1:B:476:GLY:HA3	1.95	0.47
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.49	0.47
1:A:341:VAL:HG22	1:A:342:ALA:N	2.28	0.47
1:A:60:LEU:HD12	1:A:60:LEU:C	2.35	0.47
1:A:581:ARG:NE	2:A:782:NAG:H61	2.25	0.47
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.48	0.47
1:A:458:SER:OG	1:A:471:ARG:HB2	2.15	0.47
1:B:420:ASN:ND2	1:B:426:PRO:HA	2.29	0.47
1:B:662:TYR:CZ	7:B:955:A3M:HC21	2.49	0.47
1:B:399:LYS:HB3	1:B:400:GLY:H	1.32	0.47
1:A:334:SER:CB	1:A:336:ARG:HD2	2.44	0.47
1:A:377:ASN:HB2	1:A:381:TYR:O	2.14	0.47
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.95	0.47
1:A:266:VAL:HG22	1:A:267:LYS:N	2.30	0.47
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.49	0.47
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.50	0.47
1:B:536:LYS:HG2	1:B:618:PHE:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:MET:HE3	1:B:315:TRP:C	2.34	0.47
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.80	0.47
1:A:314:GLN:NE2	1:A:359:PRO:HB2	2.30	0.47
1:B:433:LYS:HB3	1:B:445:LEU:HD21	1.96	0.47
1:B:463:LYS:HE3	9:B:1305:HOH:O	2.14	0.47
1:B:272:ASN:HD22	1:B:274:ASP:H	1.63	0.46
1:A:273:THR:HA	1:A:276:LEU:HD22	1.97	0.46
1:B:76:ILE:HG22	1:B:90:LEU:HB3	1.98	0.46
1:B:562:ASN:HB2	9:B:994:HOH:O	2.15	0.46
1:B:520:ASN:ND2	2:B:780:NAG:H4	2.31	0.46
1:B:192:ASP:O	1:B:193:ILE:HD13	2.15	0.46
1:B:544:LEU:HD21	1:B:606:GLN:HE21	1.79	0.46
1:A:420:ASN:HB2	1:A:426:PRO:HA	1.98	0.46
1:B:429:ARG:HB3	1:B:456:TYR:HA	1.98	0.46
1:A:581:ARG:NH1	2:A:782:NAG:H61	2.28	0.46
1:A:83:TYR:OH	4:A:769:FUC:H62	2.15	0.46
1:B:518:ILE:HD13	1:B:518:ILE:O	2.15	0.46
1:A:173:TYR:HB3	1:A:182:SER:OG	2.16	0.46
1:B:411:THR:HG22	9:B:1292:HOH:O	2.16	0.46
1:A:152:THR:HG23	1:A:167:VAL:O	2.16	0.46
1:A:689:MET:HG3	1:B:244:GLU:OE1	2.15	0.46
1:B:293:MET:HG2	1:B:315:TRP:HB3	1.97	0.45
3:B:778:NDG:H6C2	3:B:779:NDG:C7	2.42	0.45
1:B:236:ILE:O	1:B:253:ARG:HA	2.16	0.45
1:B:266:VAL:HG22	1:B:267:LYS:N	2.30	0.45
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.97	0.45
1:A:207:VAL:HG22	1:A:208:PHE:HD1	1.80	0.45
1:B:657:SER:HB2	1:B:689:MET:HE2	1.99	0.45
1:A:119:ASN:HD22	1:A:131:SER:CB	2.30	0.45
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.16	0.45
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.97	0.45
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.74	0.45
1:A:74:ASN:HB3	1:A:92:ASN:CG	2.36	0.45
1:A:379:GLU:O	1:A:379:GLU:HG2	2.16	0.45
2:A:780:NAG:H4	2:A:781:NAG:H2	1.77	0.45
1:A:81:ALA:O	1:A:492:ARG:NH2	2.46	0.45
1:A:74:ASN:O	1:A:92:ASN:HB3	2.17	0.45
1:A:57:LEU:HD23	9:A:1127:HOH:O	2.17	0.45
1:A:614:SER:HB3	1:A:624:ILE:HD11	1.98	0.45
1:B:599:GLY:H	1:B:602:GLU:CD	2.18	0.45
1:A:658:ARG:HD2	1:A:661:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:N	1:B:77:LEU:CD2	2.80	0.44
1:A:93:SER:CB	1:A:96:ASP:OD2	2.65	0.44
1:B:98:PHE:CE1	1:B:100:HIS:HB2	2.53	0.44
1:A:293:MET:HE2	1:A:317:ARG:HG3	1.99	0.44
1:A:369:ASN:C	1:A:389:ILE:HG23	2.37	0.44
1:A:277:SER:O	1:A:278:SER:HB3	2.17	0.44
1:B:102:ILE:HD12	1:B:116:LEU:HB3	2.00	0.44
1:B:246:LEU:HD13	1:B:248:TYR:O	2.18	0.44
3:A:770:NDG:C4	2:A:771:NAG:N2	2.76	0.44
1:B:562:ASN:OD1	1:B:564:ALA:HB3	2.17	0.44
1:B:80:ASN:OD1	1:B:82:GLU:HB3	2.17	0.44
1:B:96:ASP:O	1:B:97:GLU:HB2	2.17	0.44
1:A:286:GLN:NE2	1:A:288:THR:HG22	2.33	0.44
1:B:154:TRP:CZ2	1:B:212:SER:HB2	2.53	0.44
1:B:280:THR:CB	9:B:1091:HOH:O	2.64	0.44
1:A:76:ILE:HB	1:A:90:LEU:HD11	1.98	0.44
1:B:214:LEU:O	1:B:214:LEU:HD12	2.18	0.44
1:B:325:MET:HE1	1:B:373:LYS:HD2	1.99	0.44
1:A:161:GLY:HA3	9:A:1369:HOH:O	2.16	0.44
1:A:319:ILE:O	1:A:321:ASN:N	2.44	0.44
1:A:481:THR:OG1	1:A:483:HIS:HE1	2.01	0.44
1:A:610:ALA:HA	1:A:613:PHE:CD2	2.53	0.44
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.33	0.44
1:B:366:LEU:HB2	9:B:1371:HOH:O	2.16	0.44
1:A:651:ILE:HG23	1:A:701:LEU:HB3	1.99	0.43
1:B:744:SER:HB3	1:B:747:ALA:CB	2.48	0.43
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.53	0.43
1:B:111:GLY:O	1:B:137:LEU:HD12	2.17	0.43
1:A:386:TYR:O	1:A:394:CYS:HB2	2.19	0.43
1:A:425:MET:HA	1:A:426:PRO:HD2	1.78	0.43
1:A:408:GLU:HG3	1:A:459:VAL:CG1	2.49	0.43
1:A:546:VAL:HG22	1:A:547:TYR:N	2.32	0.43
1:A:90:LEU:CD1	1:A:90:LEU:N	2.81	0.43
1:B:309:GLU:OE1	3:B:770:NDG:O6	2.35	0.43
1:B:742:ILE:O	1:B:742:ILE:HG22	2.17	0.43
1:B:648:LYS:HE2	1:B:762:CYS:O	2.19	0.43
1:A:495:GLU:HA	9:A:1210:HOH:O	2.17	0.43
1:A:554:LYS:HB3	1:A:577:SER:HB3	2.00	0.43
1:B:218:PRO:HG2	1:B:308:GLN:OE1	2.18	0.43
1:A:704:HIS:CE1	1:A:711:VAL:O	2.71	0.43
1:B:422:TYR:C	1:B:424:GLY:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:HD2	9:B:1001:HOH:O	2.17	0.43
1:A:276:LEU:CD2	1:A:276:LEU:N	2.78	0.43
1:B:310:ARG:HD3	1:B:327:ILE:CG2	2.49	0.43
1:B:346:ILE:N	1:B:346:ILE:HD12	2.33	0.43
1:B:357:PHE:O	1:B:358:ARG:HB3	2.18	0.43
1:A:139:LYS:O	1:A:141:GLN:NE2	2.52	0.43
1:A:197:GLY:C	1:A:213:ALA:HB3	2.39	0.43
1:A:459:VAL:HG22	1:A:460:SER:N	2.33	0.43
1:A:673:LEU:HD12	1:A:673:LEU:N	2.33	0.43
2:A:775:NAG:H62	3:A:776:NDG:O	2.19	0.43
1:B:420:ASN:HD22	1:B:426:PRO:HA	1.83	0.43
1:B:58:TYR:HD1	1:B:60:LEU:CD1	2.31	0.43
1:B:75:ASN:ND2	9:B:1360:HOH:O	2.51	0.43
1:A:341:VAL:C	1:A:343:ARG:N	2.71	0.43
1:A:472:CYS:O	1:A:478:PRO:HA	2.19	0.43
1:A:651:ILE:HG23	1:A:701:LEU:HD13	2.00	0.43
1:A:314:GLN:NE2	1:A:373:LYS:HZ2	2.16	0.43
1:A:388:GLN:CB	1:A:391:LYS:HD3	2.49	0.43
2:B:780:NAG:O7	2:B:780:NAG:C3	2.67	0.43
1:A:402:TRP:HA	9:A:987:HOH:O	2.18	0.43
1:B:124:TRP:CZ2	1:B:254:VAL:HG21	2.54	0.43
1:A:203:TYR:CD2	1:A:207:VAL:CG1	3.02	0.42
1:A:285:ILE:N	1:A:285:ILE:HD12	2.33	0.42
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.54	0.42
1:B:673:LEU:HA	1:B:673:LEU:HD12	1.77	0.42
1:B:748:HIS:CE1	1:B:752:TYR:CE2	3.07	0.42
1:A:199:THR:HA	1:A:228:PHE:CE2	2.54	0.42
1:B:124:TRP:HB2	1:B:204:GLU:OE2	2.20	0.42
1:B:434:ILE:HD11	1:B:439:TYR:HA	2.01	0.42
1:B:458:SER:OG	1:B:471:ARG:HB2	2.19	0.42
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.34	0.42
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.19	0.42
2:A:775:NAG:C6	3:A:776:NDG:C1	2.97	0.42
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.54	0.42
1:A:93:SER:HB2	1:A:96:ASP:OD2	2.19	0.42
1:B:542:LEU:HD23	1:B:543:LEU:N	2.34	0.42
1:A:516:PHE:CE2	1:A:523:LYS:HE2	2.55	0.42
1:A:640:LEU:HA	1:A:640:LEU:HD23	1.85	0.42
1:A:289:ALA:HB1	1:A:290:PRO:C	2.39	0.42
1:A:402:TRP:CE3	1:A:421:GLU:HB2	2.54	0.42
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:VAL:HG22	1:B:303:VAL:O	2.19	0.42
1:A:520:ASN:OD1	2:A:782:NAG:O5	2.37	0.42
2:A:781:NAG:O7	2:A:781:NAG:H3	2.20	0.42
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.50	0.42
1:B:177:GLU:HB2	1:B:180:LEU:CG	2.49	0.42
1:B:381:TYR:CZ	1:B:401:THR:HG23	2.55	0.42
1:A:370:SER:HB2	1:A:387:PHE:O	2.20	0.42
1:A:675:THR:C	1:A:680:LEU:HB2	2.40	0.42
1:A:174:VAL:HG23	1:A:185:ILE:CG1	2.50	0.42
1:A:314:GLN:HG3	1:A:325:MET:HG3	2.01	0.42
1:A:405:ILE:N	1:A:418:ILE:O	2.50	0.41
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.02	0.41
1:A:183:TYR:HE1	1:A:277:SER:O	2.02	0.41
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.41	0.41
1:B:622:LYS:O	1:B:623:ARG:HG3	2.20	0.41
1:B:664:SER:HB2	1:B:668:GLU:OE2	2.19	0.41
2:A:775:NAG:C6	3:A:776:NDG:O	2.68	0.41
1:B:471:ARG:HH11	1:B:480:TYR:HE2	1.68	0.41
1:B:504:LEU:HA	1:B:507:VAL:HG13	2.01	0.41
1:B:548:ALA:HA	9:B:1182:HOH:O	2.21	0.41
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.90	0.41
1:B:331:ASP:OD1	1:B:333:SER:HB3	2.20	0.41
1:A:190:LYS:HA	9:A:1046:HOH:O	2.20	0.41
1:A:316:LEU:HD11	1:A:320:GLN:HA	2.02	0.41
1:A:596:ARG:N	1:A:670:TYR:O	2.49	0.41
1:A:89:PHE:O	1:A:90:LEU:HB3	2.20	0.41
1:B:139:LYS:HB3	1:B:139:LYS:HE2	1.92	0.41
1:B:459:VAL:HG22	1:B:460:SER:N	2.36	0.41
1:B:504:LEU:HD22	1:B:509:MET:HE1	1.98	0.41
1:B:535:ASP:OD1	1:B:537:SER:HB2	2.20	0.41
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.51	0.41
1:B:137:LEU:C	1:B:139:LYS:H	2.24	0.41
1:B:147:ARG:HB3	1:B:147:ARG:NH1	2.33	0.41
1:B:388:GLN:CB	1:B:391:LYS:HB2	2.50	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.19	0.41
1:A:256:TYR:CD1	1:A:256:TYR:C	2.93	0.41
1:A:314:GLN:HE22	1:A:373:LYS:HZ1	1.68	0.41
1:A:486:VAL:HG13	1:A:487:ASN:N	2.36	0.41
1:A:515:ASP:OD2	1:A:516:PHE:N	2.49	0.41
1:B:528:MET:CE	1:B:530:LEU:HD21	2.40	0.41
1:A:156:THR:HG21	1:A:214:LEU:CD1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:OD1	1:A:339:CYS:HB3	2.21	0.41
1:A:388:GLN:CB	1:A:391:LYS:HB2	2.50	0.41
1:A:388:GLN:HB2	1:A:391:LYS:HB2	2.03	0.41
1:B:675:THR:C	1:B:680:LEU:HB2	2.41	0.41
1:B:691:ARG:NH1	9:B:1156:HOH:O	2.48	0.41
1:A:208:PHE:O	1:A:209:SER:HB3	2.21	0.41
1:A:257:PRO:O	1:A:663:ASP:HA	2.20	0.41
1:B:324:VAL:HG22	1:B:346:ILE:HG13	2.02	0.41
1:B:584:GLY:O	1:B:585:TYR:HB2	2.21	0.41
1:A:336:ARG:HG2	1:A:336:ARG:HH11	1.86	0.41
1:A:658:ARG:NH1	9:A:1074:HOH:O	2.53	0.41
1:B:518:ILE:HG12	1:B:522:THR:H	1.86	0.41
1:A:118:TYR:O	1:A:119:ASN:HB2	2.21	0.41
1:A:64:SER:O	1:A:463:LYS:HG2	2.21	0.41
1:A:701:LEU:HD22	1:A:703:ILE:HG13	2.03	0.41
1:A:74:ASN:C	1:A:92:ASN:HB3	2.42	0.41
1:B:159:PRO:HD3	1:B:216:TRP:HB2	2.03	0.41
1:A:554:LYS:HB3	1:A:554:LYS:HE3	1.80	0.40
1:A:654:ALA:N	1:A:655:PRO:CD	2.84	0.40
1:A:696:LYS:CG	1:A:728:VAL:HG22	2.52	0.40
1:B:242:SER:OG	1:B:243:ASP:N	2.54	0.40
1:B:438:ASP:CG	1:B:440:THR:HG1	2.24	0.40
1:A:413:ASP:HB3	1:A:414:TYR:HD1	1.87	0.40
1:B:658:ARG:HD3	1:B:660:GLU:HB2	2.03	0.40
2:A:775:NAG:H61	3:A:776:NDG:C1	2.51	0.40
1:B:435:GLN:HB3	1:B:441:LYS:HB2	2.03	0.40
1:A:227:GLN:O	1:A:266:VAL:HA	2.22	0.40
1:A:325:MET:HE2	1:A:327:ILE:HD11	2.02	0.40
1:A:415:LEU:C	1:A:415:LEU:HD13	2.41	0.40
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.44	0.40
1:B:519:LEU:O	1:B:520:ASN:HB2	2.21	0.40
1:A:166:TYR:CE1	1:A:173:TYR:HB2	2.56	0.40
1:A:208:PHE:HE1	1:A:300:LEU:O	2.05	0.40
1:A:331:ASP:HB3	1:A:334:SER:HB2	2.02	0.40
1:A:561:LEU:HA	1:A:561:LEU:HD12	1.84	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	724/728 (100%)	661 (91%)	50 (7%)	13 (2%)	10	17
1	B	726/728 (100%)	654 (90%)	58 (8%)	14 (2%)	9	15
All	All	1450/1456 (100%)	1315 (91%)	108 (7%)	27 (2%)	9	15

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	B	289	ALA
1	B	399	LYS
1	B	645	GLY
1	B	765	LEU
1	A	289	ALA
1	A	332	GLU
1	A	389	ILE
1	A	520	ASN
1	B	85	ASN
1	B	140	ARG
1	B	280	THR
1	B	678	ASP
1	A	72	GLN
1	A	277	SER
1	A	320	GLN
1	A	521	GLU
1	B	40	ARG
1	B	87	SER
1	B	92	ASN
1	B	106	SER
1	B	423	LYS
1	A	334	SER
1	B	320	GLN
1	A	71	LYS

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Mol	Chain	Res	Type
1	A	178	PRO
1	A	161	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/653 (100%)	605 (93%)	46 (7%)	17	32
1	B	653/653 (100%)	604 (92%)	49 (8%)	16	29
All	All	1304/1306 (100%)	1209 (93%)	95 (7%)	16	31

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	51	ASN
1	A	72	GLN
1	A	90	LEU
1	A	91	GLU
1	A	92	ASN
1	A	141	GLN
1	A	145	GLU
1	A	156	THR
1	A	170	ASN
1	A	184	ARG
1	A	230	ASP
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	256	TYR
1	A	272	ASN
1	A	276	LEU
1	A	293	MET
1	A	326	ASP
1	A	336	ARG

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Mol	Chain	Res	Type
1	A	385	CYS
1	A	390	ASP
1	A	393	ASP
1	A	440	THR
1	A	448	GLU
1	A	472	CYS
1	A	482	LEU
1	A	485	SER
1	A	507	VAL
1	A	514	LEU
1	A	536	LYS
1	A	543	LEU
1	A	561	LEU
1	A	581	ARG
1	A	603	VAL
1	A	608	GLU
1	A	658	ARG
1	A	679	ASN
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	718	GLN
1	A	736	THR
1	A	760	LYS
1	A	761	GLN
1	B	41	LYS
1	B	61	ARG
1	B	66	HIS
1	B	72	GLN
1	B	75	ASN
1	B	77	LEU
1	B	125	ARG
1	B	145	GLU
1	B	147	ARG
1	B	170	ASN
1	B	184	ARG
1	B	185	ILE
1	B	209	SER
1	B	214	LEU
1	B	223	LEU
1	B	232	GLU
1	B	239	SER

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	253	ARG
1	B	272	ASN
1	B	293	MET
1	B	303	VAL
1	B	358	ARG
1	B	377	ASN
1	B	379	GLU
1	B	388	GLN
1	B	410	LEU
1	B	436	LEU
1	B	448	GLU
1	B	507	VAL
1	B	509	MET
1	B	514	LEU
1	B	517	ILE
1	B	518	ILE
1	B	522	THR
1	B	543	LEU
1	B	597	ARG
1	B	598	LEU
1	B	658	ARG
1	B	673	LEU
1	B	679	ASN
1	B	689	MET
1	B	691	ARG
1	B	701	LEU
1	B	702	LEU
1	B	710	ASN
1	B	728	VAL
1	B	760	LYS
1	B	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	72	GLN
1	A	119	ASN
1	A	123	GLN
1	A	169	ASN
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	247	GLN
1	A	272	ASN
1	A	286	GLN
1	A	314	GLN
1	A	338	ASN
1	A	388	GLN
1	A	435	GLN
1	A	483	HIS
1	A	487	ASN
1	A	505	GLN
1	A	572	ASN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	761	GLN
1	B	51	ASN
1	B	72	GLN
1	B	112	GLN
1	B	119	ASN
1	B	123	GLN
1	B	126	HIS
1	B	138	ASN
1	B	169	ASN
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	344	GLN
1	B	377	ASN
1	B	435	GLN
1	B	595	ASN
1	B	606	GLN
1	B	679	ASN
1	B	710	ASN
1	B	712	HIS
1	B	718	GLN
1	B	731	GLN
1	B	761	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	A	767	1,3,4	14,14,15	0.77	0	15,19,21	1.24	2 (13%)
3	NDG	A	768	2	14,14,15	0.87	1 (7%)	15,19,21	1.57	3 (20%)
4	FUC	A	769	2	9,10,11	0.48	0	13,14,16	0.47	0
3	NDG	A	770	1,2,4	14,14,15	0.77	0	15,19,21	0.78	1 (6%)
2	NAG	A	771	3	14,14,15	0.84	1 (7%)	15,19,21	0.63	0
4	FUC	A	772	3	9,10,11	0.58	0	13,14,16	0.48	0
2	NAG	A	773	1,2	14,14,15	0.50	0	15,19,21	0.93	0
2	NAG	A	774	2	14,14,15	0.54	0	15,19,21	0.62	0
2	NAG	A	775	1,3	14,14,15	0.59	0	15,19,21	0.87	1 (6%)
3	NDG	A	776	2,5	14,14,15	0.84	1 (7%)	15,19,21	1.27	3 (20%)
5	MAN	A	777	3	11,11,12	0.72	0	13,15,17	0.58	0
2	NAG	A	778	1,2	14,14,15	0.59	0	15,19,21	1.09	0
2	NAG	A	779	2	14,14,15	0.60	0	15,19,21	0.72	0
2	NAG	A	780	1,2	14,14,15	0.60	0	15,19,21	0.98	0
2	NAG	A	781	2	14,14,15	0.65	0	15,19,21	0.65	0
2	NAG	A	782	1	14,14,15	0.89	1 (7%)	15,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	A3M	A	954	-	10,12,12	4.19	4 (40%)	12,16,16	2.76	8 (66%)
2	NAG	B	767	1,4	14,14,15	0.62	0	15,19,21	0.79	0
4	FUC	B	768	2	9,10,11	0.54	0	13,14,16	0.46	0
2	NAG	B	769	1	14,14,15	0.63	0	15,19,21	0.82	1 (6%)
3	NDG	B	770	1,2	14,14,15	0.75	0	15,19,21	1.05	2 (13%)
2	NAG	B	771	3	14,14,15	0.55	0	15,19,21	0.60	0
2	NAG	B	772	1,2	14,14,15	0.45	0	15,19,21	0.87	1 (6%)
2	NAG	B	773	8,2	14,14,15	0.54	0	15,19,21	0.81	1 (6%)
8	BMA	B	774	2	11,11,12	0.66	0	13,15,17	0.37	0
2	NAG	B	775	1,2	14,14,15	0.63	0	15,19,21	0.82	1 (6%)
2	NAG	B	776	8,2	14,14,15	0.87	0	15,19,21	1.40	2 (13%)
8	BMA	B	777	2	11,11,12	0.74	0	13,15,17	1.08	1 (7%)
3	NDG	B	778	1,3	14,14,15	0.77	0	15,19,21	1.19	3 (20%)
3	NDG	B	779	3	14,14,15	0.76	1 (7%)	15,19,21	0.94	1 (6%)
2	NAG	B	780	1	14,14,15	0.82	0	15,19,21	0.73	1 (6%)
7	A3M	B	955	-	10,12,12	4.37	4 (40%)	12,16,16	2.67	8 (66%)

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	A	767	1,3,4	-	0/6/23/26	0/1/1/1
3	NDG	A	768	2	-	0/6/23/26	0/1/1/1
4	FUC	A	769	2	-	0/0/17/20	0/1/1/1
3	NDG	A	770	1,2,4	-	0/6/23/26	0/1/1/1
2	NAG	A	771	3	-	0/6/23/26	0/1/1/1
4	FUC	A	772	3	-	0/0/17/20	0/1/1/1
2	NAG	A	773	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	774	2	-	0/6/23/26	0/1/1/1
2	NAG	A	775	1,3	-	0/6/23/26	0/1/1/1
3	NDG	A	776	2,5	-	0/6/23/26	0/1/1/1
5	MAN	A	777	3	-	0/2/19/22	0/1/1/1
2	NAG	A	778	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	779	2	-	0/6/23/26	0/1/1/1
2	NAG	A	780	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	781	2	-	0/6/23/26	0/1/1/1
2	NAG	A	782	1	-	0/6/23/26	0/1/1/1
7	A3M	A	954	-	-	0/12/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	767	1,4	-	0/6/23/26	0/1/1/1
4	FUC	B	768	2	-	0/0/17/20	0/1/1/1
2	NAG	B	769	1	-	0/6/23/26	0/1/1/1
3	NDG	B	770	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	771	3	-	0/6/23/26	0/1/1/1
2	NAG	B	772	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	773	8,2	-	0/6/23/26	0/1/1/1
8	BMA	B	774	2	-	0/2/19/22	0/1/1/1
2	NAG	B	775	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	776	8,2	-	0/6/23/26	0/1/1/1
8	BMA	B	777	2	-	0/2/19/22	0/1/1/1
3	NDG	B	778	1,3	-	0/6/23/26	0/1/1/1
3	NDG	B	779	3	-	0/6/23/26	0/1/1/1
2	NAG	B	780	1	-	0/6/23/26	0/1/1/1
7	A3M	B	955	-	-	0/12/19/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	779	NDG	C1-C2	2.14	1.55	1.52
3	A	776	NDG	C1-C2	2.24	1.55	1.52
3	A	768	NDG	C1-C2	2.36	1.55	1.52
7	B	955	A3M	C1-C2	2.45	1.60	1.51
2	A	782	NAG	C1-C2	2.52	1.55	1.52
7	A	954	A3M	C1-C2	2.62	1.60	1.51
2	A	771	NAG	C1-C2	2.65	1.56	1.52
7	B	955	A3M	C26-C16	4.62	1.69	1.52
7	A	954	A3M	C26-C16	4.64	1.69	1.52
7	A	954	A3M	C14-N3	8.10	1.46	1.34
7	B	955	A3M	C14-N3	8.45	1.47	1.34
7	A	954	A3M	O18-C14	8.64	1.38	1.22
7	B	955	A3M	O18-C14	9.28	1.39	1.22

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	955	A3M	C4-N3-C2	-4.78	104.27	111.36
7	A	954	A3M	C4-N3-C2	-4.58	104.57	111.36
7	A	954	A3M	O18-C14-N3	-3.58	117.40	121.68
2	B	776	NAG	C4-C3-C2	-3.58	105.78	111.02
7	A	954	A3M	C2-N3-C14	-3.16	113.58	124.11
7	B	955	A3M	C2-N3-C14	-3.16	113.58	124.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	955	A3M	O18-C14-N3	-2.98	118.11	121.68
3	B	770	NDG	C4-C3-C2	-2.45	107.43	111.02
3	B	778	NDG	C2-N2-C7	-2.42	119.42	122.94
3	A	776	NDG	C4-C3-C2	-2.39	107.51	111.02
2	A	775	NAG	C2-N2-C7	-2.38	119.48	122.94
7	A	954	A3M	O18-C14-C15	-2.36	115.59	120.08
3	B	778	NDG	O-C1-C2	-2.29	108.29	111.47
2	B	775	NAG	C2-N2-C7	-2.26	119.65	122.94
2	B	773	NAG	C2-N2-C7	-2.24	119.68	122.94
3	A	768	NDG	C2-N2-C7	-2.22	119.71	122.94
7	B	955	A3M	O18-C14-C15	-2.21	115.87	120.08
2	A	767	NAG	O5-C1-C2	-2.21	108.40	111.47
7	B	955	A3M	C4-N3-C14	-2.20	116.77	124.11
3	B	779	NDG	C2-N2-C7	-2.18	119.76	122.94
7	A	954	A3M	C4-N3-C14	-2.15	116.93	124.11
7	B	955	A3M	C1-C5-C4	-2.15	99.11	105.28
3	B	770	NDG	C2-N2-C7	-2.10	119.88	122.94
7	A	954	A3M	C1-C5-C4	-2.04	99.41	105.28
2	B	772	NAG	C2-N2-C7	-2.03	119.98	122.94
3	A	770	NDG	C2-N2-C7	-2.02	119.99	122.94
2	B	769	NAG	C2-N2-C7	-2.02	120.00	122.94
3	A	776	NDG	C1-O-C5	2.00	114.92	112.17
2	B	780	NAG	C1-O5-C5	2.01	114.94	112.17
2	B	776	NAG	O4-C4-C5	2.05	114.46	109.28
3	A	776	NDG	O4-C4-C5	2.06	114.47	109.28
3	B	778	NDG	C4-C3-C2	2.42	114.57	111.02
2	A	767	NAG	C4-C3-C2	2.84	115.18	111.02
3	A	768	NDG	C1-O-C5	2.86	116.11	112.17
8	B	777	BMA	C1-C2-C3	2.95	113.39	109.65
7	B	955	A3M	C15-C14-N3	3.10	126.01	118.54
7	A	954	A3M	C15-C14-N3	3.51	127.01	118.54
7	B	955	A3M	C16-C15-C14	3.83	118.37	110.67
7	A	954	A3M	C16-C15-C14	3.86	118.43	110.67
3	A	768	NDG	O-C1-C2	4.25	117.39	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	767	NAG	2	0
3	A	768	NDG	2	0
4	A	769	FUC	1	0
3	A	770	NDG	6	0
2	A	771	NAG	6	0
4	A	772	FUC	1	0
2	A	775	NAG	6	0
3	A	776	NDG	9	0
5	A	777	MAN	3	0
2	A	779	NAG	1	0
2	A	780	NAG	1	0
2	A	781	NAG	2	0
2	A	782	NAG	8	0
7	A	954	A3M	2	0
2	B	767	NAG	1	0
4	B	768	FUC	1	0
3	B	770	NDG	3	0
2	B	771	NAG	1	0
8	B	777	BMA	1	0
3	B	778	NDG	5	0
3	B	779	NDG	5	0
2	B	780	NAG	4	0
7	B	955	A3M	3	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 ⓘ

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	726/728 (99%)	-0.18	11 (1%) 74 75	14, 30, 54, 65	0
1	B	728/728 (100%)	-0.03	23 (3%) 48 51	13, 31, 61, 88	0
All	All	1454/1456 (99%)	-0.10	34 (2%) 61 63	13, 31, 58, 88	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	SER	6.8
1	B	39	SER	6.0
1	A	279	VAL	4.8
1	A	73	GLU	3.8
1	B	97	GLU	3.7
1	B	73	GLU	3.6
1	B	333	SER	3.5
1	B	766	PRO	3.4
1	A	121	VAL	3.3
1	B	93	SER	3.1
1	B	518	ILE	2.9
1	B	40	ARG	2.9
1	B	521	GLU	2.9
1	B	75	ASN	2.8
1	B	92	ASN	2.8
1	B	88	VAL	2.8
1	B	529	ILE	2.8
1	A	278	SER	2.7
1	A	40	ARG	2.6
1	B	765	LEU	2.5
1	B	72	GLN	2.5
1	B	452	GLU	2.5
1	A	342	ALA	2.5
1	B	334	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	165	ALA	2.4
1	B	138	ASN	2.4
1	B	538	LYS	2.4
1	B	96	ASP	2.3
1	B	121	VAL	2.3
1	A	277	SER	2.3
1	A	390	ASP	2.2
1	B	471	ARG	2.2
1	A	520	ASN	2.2
1	B	330	TYR	2.2

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](#)

There are no carbohydrates in this entry.

6.4 Ligands [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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NDG	B	778	14/15	0.80	0.31	8.00	52,54,57,60	0
2	NAG	B	780	14/15	0.80	0.36	6.04	60,62,63,63	0
2	NAG	A	767	14/15	0.89	0.26	5.27	59,60,62,64	0
2	NAG	A	774	14/15	0.79	0.39	4.17	56,58,59,59	0
2	NAG	B	771	14/15	0.84	0.38	2.45	58,60,60,61	0
2	NAG	A	780	14/15	0.85	0.23	1.70	56,59,60,63	0
7	A3M	B	955	12/12	0.95	0.17	1.13	22,23,24,24	0
2	NAG	B	775	14/15	0.94	0.15	1.12	39,41,42,44	0
7	A3M	A	954	12/12	0.95	0.15	0.91	18,19,19,19	0
2	NAG	B	772	14/15	0.91	0.17	0.42	39,40,44,48	0
2	NAG	A	775	14/15	0.89	0.15	0.26	50,52,55,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	767	14/15	0.85	0.17	-0.70	68,69,71,72	0
6	HG	A	951	1/1	1.00	0.04	-3.24	36,36,36,36	0
6	HG	B	952	1/1	0.99	0.06	-4.48	36,36,36,36	0
3	NDG	A	768	14/15	0.67	0.38	-	65,66,67,67	0
2	NAG	A	782	14/15	0.70	0.52	-	63,65,66,66	0
6	HG	A	950	1/1	0.99	0.03	-	56,56,56,56	0
5	MAN	A	777	11/12	0.56	0.49	-	71,72,72,73	0
6	HG	B	953	1/1	0.99	0.03	-	60,60,60,60	0
2	NAG	B	776	14/15	0.90	0.16	-	46,47,49,51	0
8	BMA	B	774	11/12	0.77	0.34	-	58,59,59,59	0
3	NDG	A	776	14/15	0.70	0.35	-	63,65,66,69	0
2	NAG	B	769	14/15	0.81	0.36	-	62,64,64,64	0
8	BMA	B	777	11/12	0.86	0.23	-	53,54,55,55	0
3	NDG	B	770	14/15	0.89	0.25	-	50,52,54,56	0
2	NAG	A	773	14/15	0.89	0.23	-	48,49,51,54	0
3	NDG	A	770	14/15	0.74	0.51	-	70,73,77,78	0
2	NAG	A	771	14/15	0.67	0.62	-	78,80,80,80	0
2	NAG	B	773	14/15	0.83	0.31	-	51,53,54,56	0
2	NAG	A	781	14/15	0.72	0.40	-	63,65,65,66	0
3	NDG	B	779	14/15	0.75	0.55	-	62,64,65,65	0
4	FUC	B	768	10/11	0.68	0.41	-	73,73,73,73	0
4	FUC	A	769	10/11	0.91	0.31	-	63,63,63,64	0
2	NAG	A	779	14/15	0.81	0.34	-	69,70,70,70	0
4	FUC	A	772	10/11	0.76	0.57	-	79,80,80,80	0
2	NAG	A	778	14/15	0.83	0.19	-	64,65,66,67	0

6.5 Other polymers

There are no such residues in this entry.