



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:13 AM GMT

PDB ID : 1J5Q
Title : The Structure and Evolution of the Major Capsid Protein of a Large, Lipid-containing, DNA virus.
Authors : Nandhagopal, N.; Simpson, A.A.; Gurnon, J.R.; Yan, X.; Baker, T.S.; Graves, M.V.; Van Etten, J.L.; Rossmann, M.G.
Deposited on : 2002-06-27
Resolution : 2.55 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>

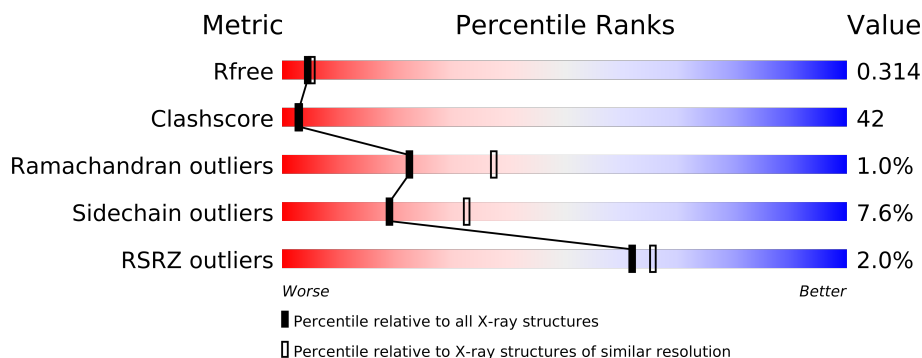
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.55 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	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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. 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	437	
1	B	437	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	438	-	X
2	NAG	B	538	-	X
2	NAG	B	546	-	X
2	NAG	B	549	-	X
3	MAN	A	439	-	X
3	MAN	A	452	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	NDG	A	446	-	X
4	NDG	A	449	-	X

2 Entry composition i

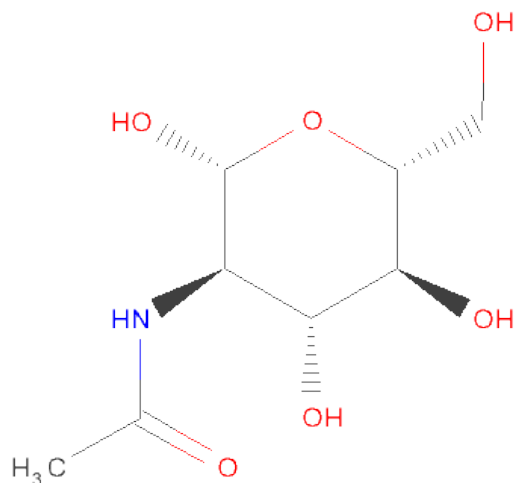
There are 6 unique types of molecules in this entry. The entry contains 6956 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3232	2052	549	623	8			
1	B	413	Total	C	N	O	S	0	0	0
			3232	2052	549	623	8			

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



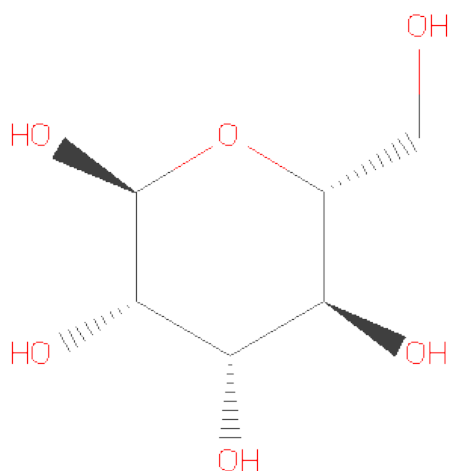
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



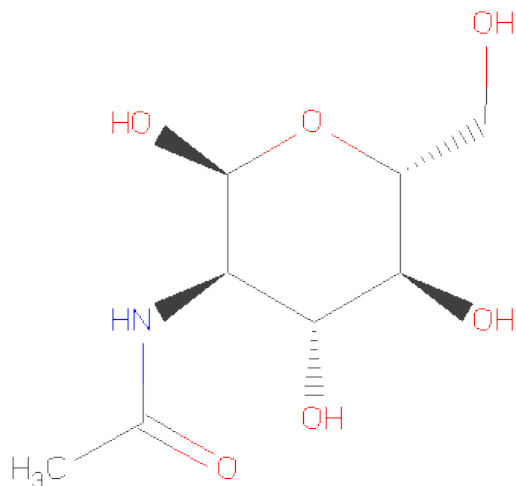
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 6 is water.

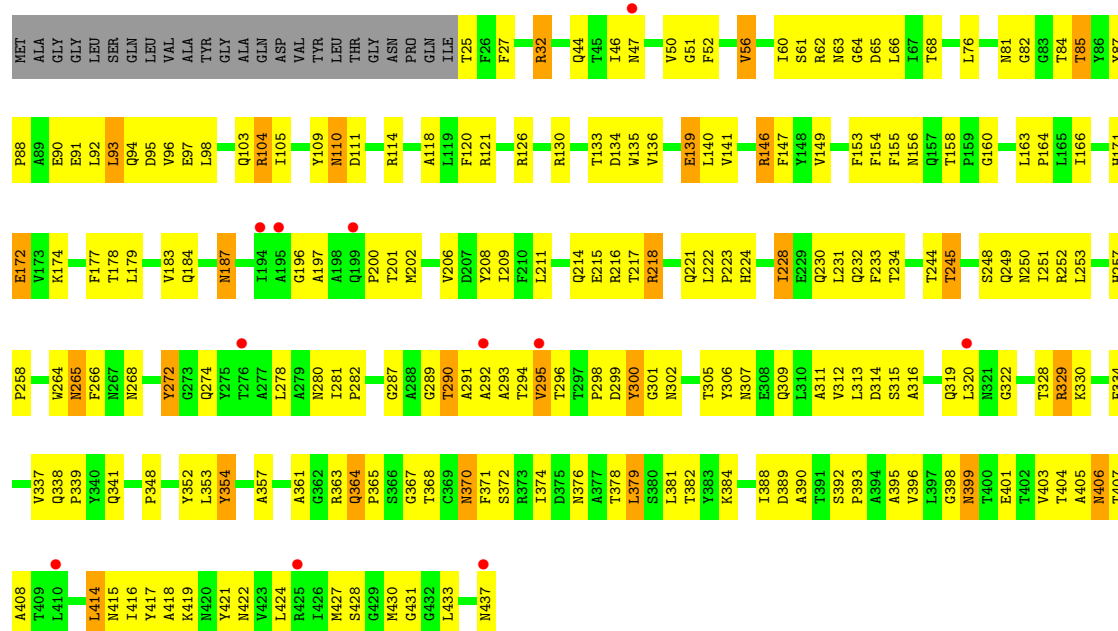
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	27	Total	O	0	0
			27	27		

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.

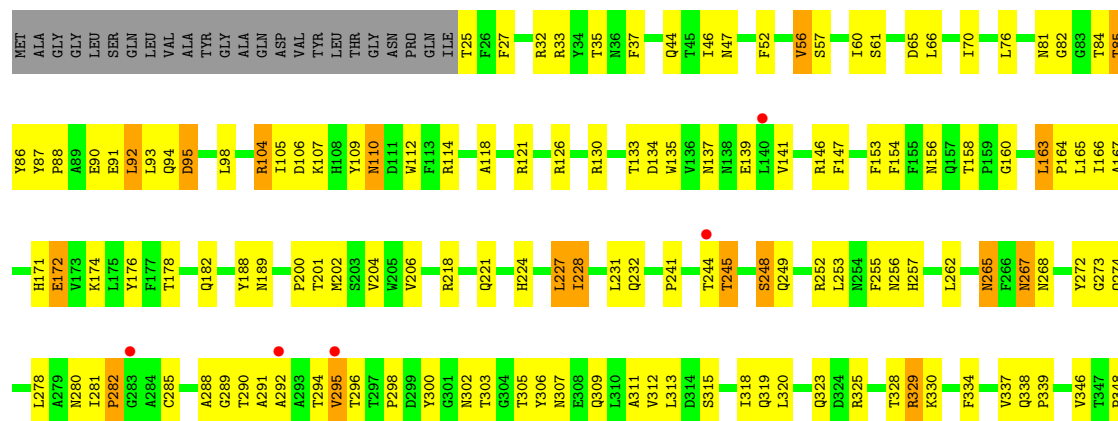
• Molecule 1: Major capsid protein

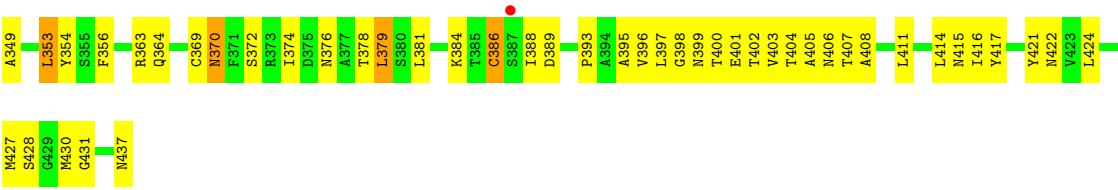
Chain A: 



• Molecule 1: Major capsid protein

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	188.76 Å 188.76 Å 188.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.42 – 2.55 84.42 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.4 (84.42-2.55) 99.6 (84.42-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.87 (at 2.55 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.269 , 0.309 0.273 , 0.314	Depositor DCC
R_{free} test set	1518 reflections (4.12%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 21.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 71863 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6956	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: HG, NAG, NDG, 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	0.39	0/3307	0.65	0/4506
1	B	0.40	0/3307	0.65	1/4506 (0.0%)
All	All	0.40	0/6614	0.65	1/9012 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	189	ASN	N-CA-C	-5.28	96.74	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	TYR	Sidechain

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	3232	0	3127	237	0
1	B	3232	0	3129	211	0
2	A	45	0	45	45	0
2	B	45	0	45	55	0
3	A	144	0	144	58	0
3	B	144	0	144	66	0
4	A	30	0	30	30	0
4	B	30	0	30	17	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	23	0	0	1	0
6	B	27	0	0	1	0
All	All	6956	0	6694	570	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 42.

All (570) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:389:ASP:H	4:A:449:NDG:H8C3	1.03	1.16
1:A:393:PRO:HG2	2:A:438:NAG:H82	1.19	1.15
2:B:538:NAG:H3	3:B:540:MAN:H2	1.26	1.13
1:B:389:ASP:H	2:B:549:NAG:H81	1.10	1.11
3:A:443:MAN:H1	3:A:447:MAN:O2	1.53	1.08
1:B:302:ASN:ND2	2:B:546:NAG:H61	1.67	1.08
2:B:538:NAG:C3	3:B:540:MAN:H2	1.85	1.07
1:A:280:ASN:HD21	2:A:438:NAG:C1	1.69	1.05
2:A:438:NAG:O3	3:A:440:MAN:H2	1.59	1.01
3:A:443:MAN:H1	2:A:444:NAG:O4	1.62	1.00
1:B:395:ALA:HB1	2:B:549:NAG:H82	1.44	0.99
1:A:399:ASN:HD21	4:A:449:NDG:H1	1.28	0.99
1:A:294:THR:HG22	1:A:295:VAL:H	1.27	0.97
1:A:280:ASN:HD21	2:A:438:NAG:H1	1.25	0.96
3:A:441:MAN:O4	3:A:442:MAN:H1	1.66	0.95
2:A:444:NAG:H61	4:A:446:NDG:O4	1.64	0.95
1:B:135:TRP:CD1	1:B:139:GLU:HG3	2.01	0.94
1:B:290:THR:HG22	1:B:292:ALA:H	1.28	0.94
3:A:447:MAN:H4	3:A:448:MAN:O1	1.68	0.94
1:B:302:ASN:HD21	2:B:546:NAG:H61	1.31	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:399:ASN:HD21	4:A:449:NDG:C1	1.81	0.93
2:A:438:NAG:HO3	3:A:440:MAN:H2	1.32	0.92
1:B:406:ASN:HD21	4:B:550:NDG:HA	0.95	0.90
1:A:389:ASP:N	4:A:449:NDG:H8C3	1.85	0.90
3:A:443:MAN:H1	3:A:447:MAN:HO2	1.30	0.89
1:A:389:ASP:H	4:A:449:NDG:C8	1.87	0.88
2:B:538:NAG:H3	3:B:540:MAN:C2	2.03	0.88
3:B:541:MAN:O4	3:B:542:MAN:H5	1.73	0.88
2:B:549:NAG:C6	3:B:553:MAN:H5	2.04	0.88
1:A:135:TRP:HB3	1:A:139:GLU:HG3	1.56	0.87
1:A:171:HIS:HD2	1:A:431:GLY:H	1.22	0.87
1:B:82:GLY:H	3:B:543:MAN:C6	1.88	0.86
1:A:290:THR:HG23	1:A:292:ALA:H	1.38	0.86
3:A:447:MAN:H61	3:A:448:MAN:H5	1.57	0.86
1:B:389:ASP:N	2:B:549:NAG:H81	1.91	0.86
1:B:81:ASN:HB3	3:B:543:MAN:H61	1.56	0.85
1:B:294:THR:HG22	1:B:295:VAL:H	1.38	0.85
1:B:406:ASN:ND2	4:B:550:NDG:HA	1.74	0.84
2:B:538:NAG:HO6	3:B:541:MAN:H2	1.41	0.84
1:B:353:LEU:HD22	1:B:354:TYR:N	1.92	0.84
1:A:406:ASN:HD22	1:A:407:THR:N	1.76	0.83
1:A:393:PRO:CG	2:A:438:NAG:H82	2.05	0.82
1:B:289:GLY:HA2	2:B:538:NAG:O7	1.79	0.82
1:A:158:THR:HG22	1:A:160:GLY:H	1.43	0.82
2:A:438:NAG:O3	3:A:440:MAN:C2	2.27	0.82
1:B:294:THR:HG22	1:B:296:THR:H	1.45	0.81
1:B:46:ILE:HG23	1:B:56:VAL:HG21	1.62	0.81
1:A:393:PRO:HG2	2:A:438:NAG:C8	2.07	0.81
1:A:183:VAL:H	1:A:187:ASN:HD21	1.28	0.81
1:A:244:THR:O	1:A:245:THR:HG22	1.81	0.81
1:A:25:THR:HG22	1:A:27:PHE:H	1.44	0.81
1:A:90:GLU:HB2	1:A:133:THR:HG21	1.63	0.81
1:A:217:THR:O	1:A:221:GLN:HG2	1.80	0.80
1:A:44:GLN:HE22	1:A:61:SER:H	1.28	0.80
1:B:389:ASP:H	2:B:549:NAG:C8	1.92	0.79
2:A:444:NAG:H4	3:A:447:MAN:O1	1.83	0.79
3:A:443:MAN:C1	2:A:444:NAG:O4	2.29	0.79
3:B:547:MAN:O4	3:B:548:MAN:H1	1.81	0.79
3:B:543:MAN:H2	3:B:545:MAN:H1	1.64	0.79
1:A:384:LYS:HD2	1:A:404:THR:HG23	1.65	0.79
1:B:384:LYS:HD2	1:B:404:THR:HG23	1.65	0.78
1:B:82:GLY:H	3:B:543:MAN:H61	1.46	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:46:ILE:CG2	1:B:56:VAL:HG21	2.13	0.78
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.49	0.78
2:B:538:NAG:C4	3:B:540:MAN:H2	2.13	0.78
1:B:171:HIS:CD2	1:B:431:GLY:H	2.01	0.78
1:B:305:THR:HG22	1:B:307:ASN:H	1.48	0.77
1:A:305:THR:HG22	1:A:307:ASN:H	1.48	0.77
1:B:91:GLU:HA	1:B:110:ASN:OD1	1.84	0.77
1:B:302:ASN:HD21	2:B:546:NAG:C6	1.98	0.77
1:B:46:ILE:HD13	1:B:202:MET:HE2	1.67	0.77
1:A:319:GLN:HE21	1:A:322:GLY:HA2	1.49	0.77
1:B:312:VAL:HG12	1:B:408:ALA:HB1	1.68	0.76
1:B:56:VAL:HG11	1:B:202:MET:HE1	1.67	0.76
2:B:538:NAG:O3	3:B:541:MAN:H2	1.85	0.76
2:B:538:NAG:C8	3:B:552:MAN:H5	2.14	0.76
1:A:278:LEU:HD21	1:A:298:PRO:HB3	1.68	0.76
3:A:443:MAN:C1	2:A:444:NAG:HO4	1.99	0.75
1:A:65:ASP:HB3	1:A:166:ILE:HD13	1.69	0.75
1:B:384:LYS:HD2	1:B:404:THR:CG2	2.17	0.75
4:B:544:NDG:O3	3:B:547:MAN:H4	1.87	0.75
3:B:543:MAN:HO3	3:B:545:MAN:C5	1.98	0.75
1:B:171:HIS:HD2	1:B:431:GLY:H	1.34	0.75
1:A:280:ASN:ND2	2:A:438:NAG:C1	2.49	0.75
1:A:257:HIS:CE1	1:A:437:ASN:HB2	2.23	0.74
3:B:539:MAN:H62	3:B:541:MAN:H3	1.68	0.74
1:B:174:LYS:HB3	1:B:174:LYS:HZ3	1.53	0.74
1:B:65:ASP:HA	1:B:166:ILE:HG23	1.70	0.74
1:A:311:ALA:O	1:A:404:THR:HG21	1.88	0.73
2:B:549:NAG:H61	3:B:553:MAN:H61	1.69	0.73
1:A:330:LYS:HE2	1:A:401:GLU:OE1	1.89	0.73
1:B:257:HIS:NE2	1:B:437:ASN:HB2	2.03	0.73
1:A:294:THR:HG22	1:A:296:THR:H	1.52	0.73
3:B:541:MAN:H61	3:B:542:MAN:O6	1.89	0.72
1:A:171:HIS:CD2	1:A:431:GLY:H	2.05	0.72
1:B:406:ASN:ND2	4:B:550:NDG:H1	2.04	0.72
2:A:438:NAG:H81	3:A:452:MAN:H5	1.71	0.72
1:B:280:ASN:ND2	2:B:538:NAG:C1	2.52	0.72
1:B:265:ASN:HD21	1:B:415:ASN:HD22	1.38	0.72
1:A:47:ASN:O	1:A:56:VAL:HG22	1.89	0.72
1:A:388:ILE:HG23	4:A:449:NDG:H8C1	1.71	0.72
1:B:90:GLU:HB2	1:B:133:THR:HG21	1.70	0.72
1:B:280:ASN:ND2	2:B:538:NAG:H1	2.05	0.71
1:B:153:PHE:H	1:B:156:ASN:HD22	1.38	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:290:THR:CG2	1:A:292:ALA:H	2.02	0.71
2:A:438:NAG:C8	3:A:452:MAN:H5	2.20	0.71
1:B:47:ASN:O	1:B:56:VAL:HG23	1.91	0.71
1:A:399:ASN:ND2	4:A:449:NDG:C1	2.53	0.70
1:B:46:ILE:HG23	1:B:56:VAL:CG2	2.21	0.70
2:A:444:NAG:C6	4:A:446:NDG:O4	2.38	0.70
2:A:438:NAG:H4	3:A:441:MAN:H2	1.72	0.70
1:A:278:LEU:HB2	1:A:407:THR:HG21	1.74	0.70
1:B:174:LYS:NZ	1:B:174:LYS:HB3	2.07	0.70
1:B:66:LEU:HD23	1:B:164:PRO:HA	1.72	0.70
1:B:280:ASN:HD21	2:B:538:NAG:C1	2.05	0.70
3:B:543:MAN:H2	3:B:545:MAN:C1	2.21	0.69
1:B:88:PRO:HD2	1:B:134:ASP:CB	2.23	0.69
3:B:541:MAN:HO4	3:B:542:MAN:H5	1.56	0.69
3:A:452:MAN:O6	3:A:452:MAN:H1	1.92	0.68
1:A:218:ARG:HH21	1:A:224:HIS:CE1	2.12	0.68
2:A:438:NAG:O3	3:A:441:MAN:O2	2.06	0.68
3:A:443:MAN:C1	3:A:447:MAN:O2	2.37	0.68
1:B:104:ARG:HG3	1:B:104:ARG:O	1.93	0.68
1:A:312:VAL:HG12	1:A:408:ALA:HB1	1.75	0.67
1:B:280:ASN:HD22	1:B:393:PRO:HG3	1.58	0.67
1:A:153:PHE:H	1:A:156:ASN:HD22	1.42	0.67
1:A:52:PHE:CE2	1:A:200:PRO:HD3	2.29	0.67
1:B:98:LEU:HD12	1:B:105:ILE:HB	1.75	0.67
1:B:88:PRO:HD2	1:B:134:ASP:HB3	1.77	0.67
1:A:289:GLY:HA2	2:A:438:NAG:O1	1.95	0.67
4:B:544:NDG:O	2:B:546:NAG:O4	2.12	0.67
1:A:25:THR:HG22	1:A:27:PHE:N	2.10	0.67
2:A:438:NAG:C4	3:A:441:MAN:H2	2.25	0.67
2:B:549:NAG:H61	3:B:553:MAN:H5	1.74	0.67
1:B:163:LEU:HD22	1:B:164:PRO:HD2	1.76	0.66
2:B:538:NAG:H3	3:B:541:MAN:O2	1.95	0.66
2:B:549:NAG:H62	3:B:553:MAN:H5	1.76	0.66
1:A:294:THR:O	1:A:295:VAL:HG23	1.96	0.66
1:A:329:ARG:HB3	1:A:329:ARG:HH11	1.61	0.66
1:B:320:LEU:HD11	1:B:325:ARG:HD3	1.77	0.66
1:B:320:LEU:HD22	1:B:374:ILE:HD13	1.76	0.66
1:B:414:LEU:HD22	1:B:416:ILE:HG13	1.78	0.66
1:B:44:GLN:NE2	1:B:60:ILE:HA	2.11	0.66
1:B:399:ASN:HD21	2:B:549:NAG:C1	2.09	0.66
1:A:379:LEU:HD13	1:A:381:LEU:HD21	1.78	0.66
3:A:443:MAN:H2	3:A:445:MAN:H1	1.79	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:82:GLY:H	3:B:543:MAN:H62	1.58	0.65
1:A:68:THR:HG23	1:A:209:ILE:HD13	1.78	0.65
1:A:294:THR:HG22	1:A:295:VAL:N	2.08	0.65
1:A:312:VAL:CG1	1:A:408:ALA:HB1	2.26	0.65
1:A:329:ARG:NH1	1:A:329:ARG:HB3	2.12	0.65
1:B:244:THR:O	1:B:245:THR:HG22	1.97	0.65
1:A:399:ASN:ND2	4:A:449:NDG:H1	2.08	0.64
1:A:251:ILE:HD12	1:A:251:ILE:N	2.12	0.64
1:B:353:LEU:HD22	1:B:354:TYR:H	1.59	0.64
3:A:447:MAN:C4	3:A:448:MAN:O1	2.45	0.64
3:A:447:MAN:H4	3:A:448:MAN:HO1	1.63	0.63
1:B:46:ILE:HD13	1:B:202:MET:CE	2.28	0.63
1:B:338:GLN:HB3	1:B:353:LEU:HD13	1.81	0.63
3:B:540:MAN:H3	3:B:541:MAN:O2	1.98	0.63
1:A:187:ASN:H	1:A:187:ASN:HD22	1.46	0.63
1:A:302:ASN:ND2	4:A:446:NDG:O	2.31	0.63
1:A:395:ALA:HB1	4:A:449:NDG:C8	2.29	0.62
1:B:44:GLN:HE21	1:B:60:ILE:HA	1.64	0.62
3:B:541:MAN:C6	3:B:542:MAN:HO6	2.13	0.62
1:B:388:ILE:HA	2:B:549:NAG:O7	2.00	0.62
1:A:309:GLN:O	1:A:404:THR:HG22	2.00	0.62
1:B:329:ARG:NH1	1:B:329:ARG:HB3	2.13	0.62
1:A:135:TRP:CD1	1:A:139:GLU:HG3	2.35	0.61
2:B:538:NAG:C3	3:B:541:MAN:O2	2.48	0.61
1:B:44:GLN:HE22	1:B:61:SER:H	1.48	0.61
1:B:290:THR:HG22	1:B:292:ALA:N	2.09	0.61
4:A:449:NDG:O3	3:A:454:MAN:O5	2.17	0.61
4:B:544:NDG:HB	3:B:547:MAN:C5	2.13	0.61
1:A:153:PHE:H	1:A:156:ASN:ND2	1.98	0.61
1:B:320:LEU:CD1	1:B:325:ARG:HD3	2.31	0.61
1:B:400:THR:HG22	1:B:402:THR:H	1.65	0.61
1:B:25:THR:HG22	1:B:27:PHE:H	1.65	0.61
3:A:447:MAN:C6	3:A:448:MAN:O1	2.49	0.60
1:B:311:ALA:O	1:B:404:THR:HG21	2.00	0.60
1:B:267:ASN:HB2	1:B:274:GLN:O	2.01	0.60
1:B:135:TRP:HD1	1:B:139:GLU:HG3	1.64	0.60
1:A:118:ALA:HB1	1:A:348:PRO:HD2	1.83	0.60
1:B:232:GLN:HE22	1:B:255:PHE:HA	1.66	0.60
1:A:280:ASN:O	1:A:393:PRO:HG3	2.01	0.60
1:B:281:ILE:HG23	1:B:282:PRO:HD2	1.82	0.60
1:B:395:ALA:CB	2:B:549:NAG:H82	2.26	0.60
1:A:395:ALA:HB1	4:A:449:NDG:H8C1	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:538:NAG:H81	3:B:552:MAN:H5	1.84	0.60
1:A:135:TRP:CB	1:A:139:GLU:HG3	2.30	0.60
1:A:25:THR:CG2	1:A:27:PHE:H	2.15	0.60
1:A:46:ILE:HD13	1:A:202:MET:HG2	1.84	0.60
1:B:280:ASN:HD21	2:B:538:NAG:H1	1.66	0.60
2:A:444:NAG:O5	4:A:446:NDG:O4	2.20	0.60
1:A:257:HIS:NE2	1:A:437:ASN:HB2	2.16	0.60
4:A:449:NDG:O4	3:A:453:MAN:O1	2.14	0.60
1:A:337:VAL:O	1:A:341:GLN:HG3	2.01	0.60
1:A:44:GLN:NE2	1:A:60:ILE:HA	2.16	0.59
1:B:87:TYR:N	1:B:88:PRO:HD3	2.17	0.59
1:A:82:GLY:H	3:A:443:MAN:C6	2.15	0.59
1:B:280:ASN:O	1:B:280:ASN:ND2	2.35	0.59
2:B:549:NAG:O1	2:B:549:NAG:C7	2.50	0.59
1:B:218:ARG:HH21	1:B:224:HIS:CE1	2.20	0.59
1:A:258:PRO:HB3	1:A:368:THR:HG21	1.85	0.59
1:A:299:ASP:O	1:A:301:GLY:N	2.36	0.59
1:A:312:VAL:O	1:A:384:LYS:HG3	2.03	0.59
1:A:265:ASN:C	1:A:265:ASN:HD22	2.05	0.59
1:A:257:HIS:NE2	1:A:437:ASN:C	2.56	0.59
3:A:439:MAN:O5	3:A:441:MAN:O3	2.21	0.58
1:A:62:ARG:NH2	1:A:166:ILE:HA	2.18	0.58
2:B:538:NAG:O4	3:B:540:MAN:H2	2.02	0.58
1:B:98:LEU:CD1	1:B:105:ILE:HB	2.33	0.58
1:B:121:ARG:HG2	1:B:126:ARG:HA	1.84	0.58
1:A:231:LEU:HD13	1:A:232:GLN:N	2.18	0.58
1:A:274:GLN:NE2	1:A:278:LEU:HG	2.18	0.58
3:B:547:MAN:O6	3:B:548:MAN:H1	2.03	0.58
1:A:94:GLN:HA	1:A:110:ASN:ND2	2.19	0.58
3:A:452:MAN:O6	3:A:452:MAN:C1	2.50	0.58
1:B:81:ASN:OD1	1:B:141:VAL:HG23	2.03	0.58
1:A:95:ASP:OD1	1:A:178:THR:HB	2.04	0.58
1:B:399:ASN:ND2	2:B:549:NAG:O1	2.27	0.58
1:A:98:LEU:HD12	1:A:105:ILE:HB	1.84	0.58
1:B:232:GLN:NE2	1:B:255:PHE:HA	2.18	0.57
2:B:549:NAG:H61	3:B:553:MAN:C6	2.34	0.57
1:A:65:ASP:HB3	1:A:166:ILE:CD1	2.33	0.57
1:A:85:THR:HG23	1:A:88:PRO:HD3	1.84	0.57
1:B:330:LYS:HE2	1:B:401:GLU:OE1	2.03	0.57
1:A:314:ASP:HB3	1:A:382:THR:O	2.04	0.57
3:A:439:MAN:C1	3:A:441:MAN:O3	2.51	0.57
1:A:120:PHE:HD2	1:A:361:ALA:HB2	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:302:ASN:HD21	2:B:546:NAG:C5	2.18	0.57
1:B:338:GLN:HB2	1:B:339:PRO:HD3	1.86	0.57
1:A:281:ILE:HG23	1:A:282:PRO:HD2	1.87	0.57
1:B:82:GLY:N	3:B:543:MAN:H62	2.20	0.57
1:A:130:ARG:HG2	1:A:136:VAL:CG1	2.35	0.57
1:B:370:ASN:ND2	1:B:372:SER:H	2.03	0.57
1:A:218:ARG:NH2	1:A:224:HIS:CE1	2.73	0.57
1:B:329:ARG:HH11	1:B:329:ARG:HB3	1.69	0.57
1:B:290:THR:CG2	1:B:291:ALA:N	2.68	0.56
1:A:280:ASN:HD22	1:A:393:PRO:HD3	1.70	0.56
3:B:541:MAN:H61	3:B:542:MAN:HO6	1.70	0.56
1:B:52:PHE:CE2	1:B:200:PRO:HD3	2.40	0.56
4:A:449:NDG:HC	3:A:453:MAN:HO1	1.49	0.56
2:B:538:NAG:O3	3:B:541:MAN:C2	2.52	0.56
1:A:302:ASN:HD21	4:A:446:NDG:C5	2.18	0.56
1:B:406:ASN:CG	4:B:550:NDG:H1	2.26	0.56
1:B:281:ILE:HD13	1:B:397:LEU:HD21	1.87	0.56
2:B:538:NAG:H82	3:B:552:MAN:H5	1.86	0.56
3:B:547:MAN:O4	3:B:548:MAN:C1	2.51	0.56
1:A:93:LEU:HD21	1:A:177:PHE:HD2	1.70	0.56
1:A:172:GLU:OE1	1:A:174:LYS:HD2	2.05	0.56
2:B:538:NAG:H3	3:B:540:MAN:C1	2.35	0.56
1:A:183:VAL:H	1:A:187:ASN:ND2	2.00	0.56
2:B:538:NAG:O6	3:B:541:MAN:H2	2.02	0.56
1:A:81:ASN:HB3	3:A:443:MAN:H61	1.86	0.56
1:B:406:ASN:ND2	4:B:550:NDG:C1	2.68	0.56
1:A:88:PRO:HD2	1:A:134:ASP:CB	2.36	0.56
1:A:32:ARG:H	1:A:32:ARG:HD2	1.71	0.56
1:B:320:LEU:HG	1:B:325:ARG:HB2	1.88	0.55
1:A:305:THR:HG22	1:A:306:TYR:N	2.22	0.55
1:B:85:THR:HG23	1:B:88:PRO:HD3	1.87	0.55
1:B:257:HIS:CE1	1:B:437:ASN:HB2	2.42	0.55
1:A:66:LEU:HD23	1:A:164:PRO:HA	1.88	0.55
1:A:370:ASN:ND2	1:A:372:SER:H	2.05	0.55
1:A:290:THR:HG23	1:A:291:ALA:N	2.22	0.55
1:B:84:THR:HG22	1:B:84:THR:O	2.06	0.55
3:B:543:MAN:HO3	3:B:545:MAN:C6	2.20	0.55
1:B:295:VAL:O	1:B:295:VAL:HG12	2.07	0.55
1:A:133:THR:HG22	1:A:133:THR:O	2.06	0.55
2:B:549:NAG:H61	3:B:553:MAN:C5	2.37	0.54
2:A:444:NAG:O1	4:A:446:NDG:H5	2.07	0.54
2:A:444:NAG:C5	4:A:446:NDG:HC	2.19	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:440:MAN:H2	3:A:441:MAN:O2	2.08	0.54
1:B:398:GLY:O	2:B:549:NAG:H62	2.06	0.54
1:A:171:HIS:HD2	1:A:431:GLY:N	2.00	0.54
1:A:363:ARG:HA	1:A:363:ARG:HE	1.73	0.54
4:A:449:NDG:O7	3:A:454:MAN:H61	2.07	0.54
1:B:406:ASN:ND2	4:B:550:NDG:N2	2.44	0.54
1:B:294:THR:HG22	1:B:295:VAL:N	2.16	0.54
1:B:280:ASN:ND2	2:B:538:NAG:O1	2.40	0.54
1:B:66:LEU:CD2	1:B:164:PRO:HA	2.38	0.54
1:B:86:TYR:HE2	1:B:273:GLY:HA3	1.73	0.54
3:B:541:MAN:C6	3:B:542:MAN:O6	2.56	0.54
1:B:312:VAL:O	1:B:384:LYS:HG3	2.07	0.54
1:B:281:ILE:HD11	1:B:396:VAL:HB	1.90	0.54
1:B:82:GLY:HA3	3:B:543:MAN:H62	1.89	0.54
1:A:302:ASN:ND2	4:A:446:NDG:H6C2	2.22	0.54
1:A:320:LEU:CD2	1:A:374:ILE:HD13	2.38	0.53
1:B:280:ASN:OD1	2:B:538:NAG:O1	2.18	0.53
1:A:140:LEU:HD23	3:A:443:MAN:H61	1.90	0.53
1:A:184:GLN:HG2	1:A:300:TYR:CD2	2.43	0.53
1:A:384:LYS:HD2	1:A:404:THR:CG2	2.36	0.53
1:A:60:ILE:HD12	1:A:206:VAL:HG21	1.89	0.53
1:A:111:ASP:HB3	1:A:417:TYR:OH	2.08	0.53
1:B:319:GLN:HG3	1:B:323:GLN:O	2.08	0.53
1:A:287:GLY:O	1:A:293:ALA:HB2	2.07	0.53
1:B:158:THR:HG22	1:B:160:GLY:H	1.72	0.53
1:B:278:LEU:HD21	1:B:298:PRO:HB3	1.91	0.53
1:A:62:ARG:HH21	1:A:166:ILE:HA	1.74	0.53
1:B:379:LEU:HD12	1:B:416:ILE:CD1	2.39	0.53
2:B:549:NAG:HO3	3:B:554:MAN:C5	2.21	0.52
1:A:134:ASP:HA	1:A:147:PHE:CE2	2.44	0.52
1:B:379:LEU:HD12	1:B:416:ILE:HD11	1.90	0.52
1:A:250:ASN:C	1:A:251:ILE:HD12	2.30	0.52
1:A:230:GLN:O	1:A:419:LYS:HD2	2.09	0.52
1:B:338:GLN:HB3	1:B:353:LEU:CD1	2.39	0.52
1:A:171:HIS:CD2	1:A:430:MET:HA	2.45	0.52
3:B:543:MAN:O3	3:B:545:MAN:O6	2.26	0.52
1:A:305:THR:HG22	1:A:307:ASN:N	2.21	0.52
1:A:82:GLY:H	3:A:443:MAN:H62	1.74	0.52
1:A:94:GLN:HG3	1:A:110:ASN:ND2	2.25	0.52
1:B:94:GLN:HB3	1:B:178:THR:O	2.08	0.52
1:B:244:THR:O	1:B:245:THR:O	2.28	0.52
1:B:252:ARG:NE	1:B:376:ASN:ND2	2.57	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:438:NAG:H83	3:A:452:MAN:C5	2.40	0.52
1:B:65:ASP:HB3	1:B:166:ILE:HD13	1.91	0.52
4:B:544:NDG:O3	3:B:547:MAN:C4	2.57	0.52
1:B:118:ALA:HB1	1:B:348:PRO:HD2	1.91	0.52
1:B:265:ASN:HD22	1:B:265:ASN:C	2.14	0.52
1:B:278:LEU:HB2	1:B:407:THR:HG21	1.92	0.52
1:B:305:THR:HG22	1:B:307:ASN:N	2.22	0.51
1:A:135:TRP:CG	1:A:139:GLU:HG3	2.46	0.51
1:A:87:TYR:N	1:A:88:PRO:HD3	2.26	0.51
1:B:95:ASP:OD2	1:B:178:THR:HB	2.10	0.51
1:A:223:PRO:HB3	1:A:427:MET:HE2	1.92	0.51
1:A:146:ARG:NH1	1:A:146:ARG:HG2	2.22	0.51
1:A:364:GLN:NE2	1:A:365:PRO:O	2.44	0.51
1:B:285:CYS:SG	1:B:288:ALA:HB2	2.50	0.51
2:B:538:NAG:O6	3:B:539:MAN:H5	2.10	0.51
1:A:221:GLN:HE21	1:A:221:GLN:HA	1.75	0.51
1:A:265:ASN:C	1:A:265:ASN:ND2	2.63	0.51
4:B:544:NDG:HA	3:B:547:MAN:C6	2.24	0.51
1:B:298:PRO:HG2	1:B:300:TYR:CE2	2.45	0.51
1:A:91:GLU:HA	1:A:110:ASN:OD1	2.10	0.51
1:B:46:ILE:HD11	1:B:204:VAL:HG23	1.93	0.50
1:B:114:ARG:HD2	1:B:272:TYR:CE2	2.45	0.50
1:B:227:LEU:HD13	1:B:421:TYR:CD1	2.46	0.50
1:A:135:TRP:HB3	1:A:139:GLU:CG	2.36	0.50
1:A:81:ASN:OD1	1:A:141:VAL:HG23	2.11	0.50
1:A:46:ILE:CD1	1:A:202:MET:HG2	2.41	0.50
1:B:253:LEU:HD22	1:B:255:PHE:CE1	2.47	0.50
1:B:370:ASN:HD22	1:B:370:ASN:C	2.14	0.50
3:B:547:MAN:O6	3:B:548:MAN:C1	2.59	0.50
1:B:274:GLN:N	1:B:303:THR:HG21	2.27	0.50
1:B:94:GLN:HG2	1:B:95:ASP:OD1	2.12	0.50
1:B:137:ASN:N	1:B:139:GLU:OE2	2.40	0.50
2:A:444:NAG:C5	4:A:446:NDG:O4	2.59	0.49
1:A:130:ARG:HG2	1:A:136:VAL:HG11	1.94	0.49
1:A:395:ALA:O	1:A:399:ASN:ND2	2.44	0.49
1:B:86:TYR:CE2	1:B:303:THR:HB	2.46	0.49
1:A:281:ILE:HD11	1:A:396:VAL:HB	1.93	0.49
2:B:538:NAG:O4	2:B:538:NAG:N2	2.41	0.49
1:B:174:LYS:NZ	1:B:176:TYR:CZ	2.80	0.49
2:A:438:NAG:HO3	3:A:441:MAN:C2	2.19	0.49
2:A:438:NAG:C8	3:A:452:MAN:C5	2.88	0.49
1:B:338:GLN:HG3	1:B:353:LEU:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:LEU:HD23	1:A:164:PRO:HD2	1.94	0.49
1:A:232:GLN:HB2	1:A:418:ALA:HB3	1.95	0.49
1:A:370:ASN:HD22	1:A:370:ASN:C	2.14	0.49
1:A:103:GLN:HE22	1:A:433:LEU:HD12	1.78	0.49
1:A:44:GLN:HE21	1:A:60:ILE:HA	1.77	0.49
1:B:414:LEU:CD2	1:B:416:ILE:HG13	2.41	0.49
1:B:274:GLN:NE2	1:B:278:LEU:HG	2.27	0.49
3:A:445:MAN:H1	3:A:448:MAN:H2	1.93	0.49
1:B:221:GLN:OE1	1:B:221:GLN:HA	2.13	0.49
1:B:386:CYS:HB2	1:B:406:ASN:HA	1.93	0.48
1:A:76:LEU:CD2	1:A:200:PRO:HB3	2.43	0.48
1:A:251:ILE:O	1:A:378:THR:HG23	2.13	0.48
1:B:329:ARG:HB2	1:B:334:PHE:CE1	2.48	0.48
1:A:398:GLY:O	4:A:449:NDG:H6C2	2.13	0.48
1:B:280:ASN:CG	2:B:538:NAG:HO1	2.14	0.48
1:B:312:VAL:HG23	1:B:313:LEU:N	2.27	0.48
1:A:389:ASP:CB	4:A:449:NDG:H8C3	2.44	0.48
1:A:280:ASN:ND2	1:A:393:PRO:HD3	2.29	0.48
2:A:438:NAG:H83	3:A:452:MAN:H5	1.94	0.48
1:B:312:VAL:CG1	1:B:408:ALA:HB1	2.40	0.48
1:A:87:TYR:OH	1:A:130:ARG:HD2	2.13	0.48
1:A:97:GLU:CD	1:A:104:ARG:HH11	2.16	0.48
3:A:443:MAN:C3	3:A:445:MAN:H1	2.43	0.48
1:A:82:GLY:H	3:A:443:MAN:H61	1.79	0.48
1:B:378:THR:HG22	1:B:379:LEU:N	2.29	0.48
1:A:309:GLN:NE2	1:A:403:VAL:O	2.46	0.48
1:A:312:VAL:HG23	1:A:313:LEU:N	2.29	0.48
3:B:540:MAN:C3	3:B:541:MAN:O2	2.61	0.48
1:B:130:ARG:HG2	1:B:134:ASP:OD2	2.14	0.48
2:A:438:NAG:O4	3:A:441:MAN:C2	2.62	0.48
1:A:154:PHE:CD1	1:A:155:PHE:N	2.82	0.48
1:A:114:ARG:NE	1:A:114:ARG:HA	2.29	0.48
1:B:309:GLN:O	1:B:404:THR:HG22	2.14	0.47
1:B:280:ASN:ND2	1:B:393:PRO:HG3	2.27	0.47
2:B:549:NAG:O3	3:B:554:MAN:C1	2.62	0.47
2:A:444:NAG:O1	4:A:446:NDG:H6C1	2.14	0.47
1:A:353:LEU:HD13	1:A:354:TYR:N	2.28	0.47
1:B:379:LEU:HD13	1:B:381:LEU:HD11	1.97	0.47
1:B:82:GLY:CA	3:B:543:MAN:H62	2.44	0.47
1:B:82:GLY:HA3	4:B:544:NDG:H6C1	1.96	0.47
1:A:85:THR:CG2	1:A:134:ASP:HB2	2.45	0.47
1:A:65:ASP:CG	1:A:216:ARG:HD3	2.35	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:87:TYR:CE2	1:B:130:ARG:HG3	2.50	0.47
1:A:370:ASN:HD22	1:A:372:SER:H	1.63	0.47
1:A:51:GLY:O	1:A:179:LEU:HD12	2.13	0.47
1:A:253:LEU:HD21	1:A:416:ILE:HD13	1.95	0.47
1:B:85:THR:HG23	1:B:88:PRO:CD	2.45	0.47
1:A:388:ILE:HD11	1:A:403:VAL:HG23	1.96	0.47
1:A:65:ASP:O	1:A:166:ILE:HG12	2.15	0.47
1:A:320:LEU:HD21	1:A:374:ILE:HD13	1.96	0.47
1:A:218:ARG:HH21	1:A:224:HIS:HE1	1.57	0.46
1:B:86:TYR:CE2	1:B:273:GLY:HA3	2.51	0.46
1:B:384:LYS:CD	1:B:404:THR:HG23	2.41	0.46
3:A:443:MAN:H3	3:A:445:MAN:H1	1.97	0.46
3:A:447:MAN:H61	3:A:448:MAN:O1	2.15	0.46
1:A:320:LEU:HD22	1:A:374:ILE:HG21	1.96	0.46
1:B:231:LEU:HD11	1:B:417:TYR:HD2	1.80	0.46
2:A:444:NAG:C4	3:A:447:MAN:O1	2.61	0.46
1:A:114:ARG:HD2	1:A:272:TYR:CE2	2.50	0.46
1:A:392:SER:O	1:A:396:VAL:HG23	2.15	0.46
1:A:302:ASN:HD21	4:A:446:NDG:H6C2	1.79	0.46
1:B:280:ASN:O	1:B:281:ILE:HG13	2.16	0.46
3:B:547:MAN:O4	3:B:548:MAN:C2	2.64	0.46
1:A:158:THR:HG22	1:A:160:GLY:N	2.20	0.46
1:A:251:ILE:CD1	1:A:251:ILE:N	2.78	0.46
1:B:388:ILE:HB	1:B:404:THR:O	2.15	0.46
2:B:538:NAG:O4	3:B:540:MAN:C2	2.64	0.46
1:A:87:TYR:HB3	1:A:90:GLU:HB3	1.97	0.46
1:B:232:GLN:HE22	1:B:256:ASN:H	1.64	0.46
1:A:93:LEU:HD12	1:A:149:VAL:HG11	1.98	0.46
1:B:88:PRO:HD2	1:B:134:ASP:HB2	1.97	0.45
1:A:338:GLN:HB2	1:A:339:PRO:HD3	1.98	0.45
2:B:538:NAG:H3	3:B:540:MAN:O1	2.16	0.45
1:A:294:THR:CG2	1:A:295:VAL:H	2.06	0.45
1:A:406:ASN:CG	2:A:450:NAG:O1	2.54	0.45
1:A:88:PRO:HD2	1:A:134:ASP:HB3	1.98	0.45
4:B:550:NDG:H8C2	3:B:551:MAN:O2	2.17	0.45
1:A:309:GLN:O	1:A:309:GLN:HG3	2.16	0.45
1:B:281:ILE:HD13	1:B:397:LEU:CD2	2.46	0.45
1:A:221:GLN:NE2	1:A:221:GLN:HA	2.32	0.45
1:B:172:GLU:OE1	1:B:174:LYS:HD2	2.16	0.45
1:A:50:VAL:HG13	1:A:202:MET:HE2	1.99	0.45
2:A:438:NAG:C4	3:A:441:MAN:C2	2.94	0.45
1:A:266:PHE:CE2	1:A:414:LEU:HG	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:538:NAG:H3	3:B:540:MAN:HO1	1.81	0.45
1:B:133:THR:O	1:B:133:THR:HG22	2.17	0.45
1:A:280:ASN:ND2	2:A:438:NAG:O5	2.50	0.45
1:A:357:ALA:HB2	1:A:367:GLY:O	2.16	0.45
1:B:309:GLN:NE2	1:B:403:VAL:O	2.50	0.44
1:A:56:VAL:HG11	1:A:202:MET:CE	2.47	0.44
1:A:265:ASN:HD21	1:A:415:ASN:HD22	1.65	0.44
1:A:338:GLN:HG3	1:A:353:LEU:O	2.17	0.44
1:B:109:TYR:O	1:B:112:TRP:HB3	2.17	0.44
1:B:305:THR:O	1:B:349:ALA:N	2.47	0.44
1:A:65:ASP:O	1:A:66:LEU:HD23	2.17	0.44
1:B:88:PRO:CD	1:B:134:ASP:CB	2.95	0.44
1:B:228:ILE:HD11	1:B:422:ASN:HB3	1.98	0.44
1:B:337:VAL:O	1:B:338:GLN:C	2.55	0.44
1:A:334:PHE:HB2	1:A:352:TYR:HB3	1.98	0.44
1:A:295:VAL:O	1:A:295:VAL:HG12	2.17	0.44
2:A:438:NAG:H83	3:A:452:MAN:O5	2.17	0.44
1:A:61:SER:OG	1:A:63:ASN:ND2	2.51	0.44
4:B:544:NDG:HA	3:B:547:MAN:H62	1.83	0.44
2:A:450:NAG:H83	3:A:451:MAN:O3	2.17	0.44
1:A:389:ASP:HB3	4:A:449:NDG:H8C3	1.99	0.44
1:B:265:ASN:ND2	1:B:265:ASN:C	2.70	0.44
1:A:121:ARG:HG2	1:A:126:ARG:HA	1.99	0.44
1:A:406:ASN:OD1	2:A:450:NAG:C1	2.66	0.44
1:A:319:GLN:HE21	1:A:322:GLY:CA	2.26	0.44
1:A:84:THR:HG22	1:A:84:THR:O	2.18	0.44
1:B:312:VAL:CG1	1:B:411:LEU:HD12	2.47	0.43
1:B:395:ALA:O	1:B:399:ASN:ND2	2.46	0.43
1:A:379:LEU:CD1	1:A:381:LEU:HD21	2.47	0.43
1:B:158:THR:OG1	1:B:363:ARG:HG3	2.18	0.43
1:A:233:PHE:CD1	1:A:234:THR:N	2.86	0.43
1:A:110:ASN:HB3	1:A:272:TYR:HE1	1.84	0.43
3:A:443:MAN:C2	3:A:445:MAN:H1	2.46	0.43
1:A:228:ILE:HD13	1:A:422:ASN:O	2.19	0.43
3:A:445:MAN:C1	3:A:448:MAN:H2	2.48	0.43
1:B:241:PRO:HB2	1:B:386:CYS:SG	2.58	0.43
1:B:52:PHE:CZ	1:B:200:PRO:HD3	2.54	0.43
1:A:365:PRO:HB3	1:A:421:TYR:CE2	2.54	0.43
1:A:390:ALA:HB2	1:A:405:ALA:HB1	2.00	0.43
1:A:293:ALA:HB3	2:A:438:NAG:O6	2.19	0.43
1:B:172:GLU:HG3	1:B:172:GLU:H	1.61	0.43
1:B:106:ASP:OD1	1:B:107:LYS:N	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:182:GLN:NE2	1:B:188:TYR:CZ	2.87	0.43
1:A:295:VAL:CG1	1:A:295:VAL:O	2.67	0.43
3:A:447:MAN:C5	3:A:448:MAN:O1	2.67	0.43
1:A:406:ASN:HD22	1:A:407:THR:H	1.58	0.43
1:A:218:ARG:HG2	1:A:222:LEU:CD1	2.49	0.43
1:A:427:MET:HG2	1:A:428:SER:H	1.84	0.43
1:A:315:SER:HB2	1:A:328:THR:CG2	2.48	0.43
1:B:56:VAL:CG2	1:B:57:SER:N	2.82	0.43
1:B:248:SER:O	1:B:249:GLN:HB2	2.19	0.43
3:A:452:MAN:O6	3:A:452:MAN:O2	2.15	0.42
3:B:547:MAN:O4	3:B:548:MAN:H2	2.19	0.42
2:B:538:NAG:C3	3:B:540:MAN:C2	2.75	0.42
1:A:299:ASP:CG	1:A:302:ASN:HD22	2.22	0.42
4:B:550:NDG:O7	3:B:551:MAN:O2	2.36	0.42
1:A:392:SER:O	1:A:395:ALA:HB3	2.18	0.42
1:A:155:PHE:CE2	1:A:163:LEU:HD12	2.54	0.42
1:A:252:ARG:NE	1:A:376:ASN:ND2	2.67	0.42
1:A:61:SER:CB	1:A:63:ASN:HD21	2.32	0.42
1:A:211:LEU:HD22	1:A:215:GLU:OE1	2.20	0.42
1:A:52:PHE:CZ	1:A:200:PRO:HD3	2.54	0.42
1:A:315:SER:O	1:A:316:ALA:HB2	2.18	0.42
1:A:264:TRP:HA	1:A:415:ASN:O	2.19	0.42
1:B:35:THR:O	1:B:37:PHE:HD2	2.02	0.42
1:A:196:GLY:O	1:A:197:ALA:C	2.57	0.42
4:B:550:NDG:O7	3:B:551:MAN:H4	2.19	0.42
1:B:329:ARG:HH11	1:B:329:ARG:CB	2.32	0.42
1:B:232:GLN:HE22	1:B:256:ASN:N	2.17	0.42
1:B:319:GLN:HG3	1:B:323:GLN:C	2.40	0.42
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.84	0.42
2:A:438:NAG:HO4	3:A:441:MAN:C2	2.33	0.42
2:B:549:NAG:C4	3:B:553:MAN:HO1	2.30	0.42
1:A:406:ASN:C	1:A:406:ASN:HD22	2.16	0.42
1:B:154:PHE:CB	1:B:228:ILE:HB	2.50	0.42
1:A:172:GLU:H	1:A:172:GLU:HG3	1.59	0.42
1:B:290:THR:CG2	1:B:292:ALA:H	2.15	0.42
1:A:158:THR:OG1	1:A:363:ARG:HG3	2.18	0.42
2:A:438:NAG:O1	2:A:438:NAG:C7	2.68	0.42
1:B:291:ALA:HA	3:B:541:MAN:O1	2.18	0.42
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.91	0.41
1:A:94:GLN:HB3	1:A:178:THR:O	2.20	0.41
1:B:262:LEU:HD12	1:B:318:ILE:CD1	2.50	0.41
1:A:221:GLN:NE2	1:A:221:GLN:CA	2.81	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:ASN:ND2	2:A:438:NAG:H1	2.10	0.41
1:A:187:ASN:N	1:A:187:ASN:HD22	2.10	0.41
1:A:287:GLY:O	1:A:290:THR:HG22	2.20	0.41
1:A:155:PHE:CD2	1:A:163:LEU:HD12	2.56	0.41
1:B:25:THR:HG22	1:B:27:PHE:N	2.34	0.41
2:A:438:NAG:C3	3:A:440:MAN:O2	2.69	0.41
1:A:302:ASN:HD21	4:A:446:NDG:C6	2.33	0.41
1:B:46:ILE:CG2	1:B:56:VAL:CG2	2.89	0.41
1:B:76:LEU:HB2	1:B:147:PHE:HE1	1.84	0.41
1:B:406:ASN:HD21	4:B:550:NDG:C1	2.34	0.41
1:A:133:THR:O	1:A:133:THR:CG2	2.69	0.41
1:A:146:ARG:NH1	1:A:146:ARG:CG	2.82	0.41
1:A:66:LEU:HD11	1:A:211:LEU:HD11	2.03	0.41
1:B:427:MET:HG2	1:B:428:SER:N	2.36	0.41
1:B:165:LEU:C	1:B:167:ALA:H	2.23	0.41
1:B:280:ASN:HA	1:B:285:CYS:SG	2.61	0.41
1:B:171:HIS:NE2	1:B:430:MET:HB3	2.36	0.41
1:B:405:ALA:C	1:B:407:THR:N	2.74	0.41
1:B:280:ASN:CG	2:B:538:NAG:O1	2.59	0.41
2:B:549:NAG:O3	3:B:554:MAN:O5	2.32	0.41
1:A:120:PHE:CD2	1:A:361:ALA:HB2	2.51	0.41
1:B:306:TYR:CD2	1:B:348:PRO:HA	2.56	0.41
1:A:103:GLN:HG2	6:A:466:HOH:O	2.21	0.41
1:B:33:ARG:NH1	1:B:33:ARG:HG3	2.36	0.41
1:A:64:GLY:HA3	1:A:208:TYR:HB3	2.03	0.41
1:A:395:ALA:CB	4:A:449:NDG:H8C2	2.51	0.41
1:B:290:THR:HG22	1:B:291:ALA:N	2.36	0.41
1:B:46:ILE:O	1:B:46:ILE:HG22	2.21	0.41
1:A:370:ASN:HD22	1:A:371:PHE:N	2.18	0.41
1:B:70:ILE:HG12	1:B:206:VAL:HG22	2.03	0.41
1:A:98:LEU:CD1	1:A:105:ILE:HB	2.49	0.40
1:B:158:THR:OG1	1:B:363:ARG:HD2	2.21	0.40
1:A:389:ASP:OD1	1:A:392:SER:N	2.54	0.40
2:A:438:NAG:HO3	3:A:440:MAN:C2	2.15	0.40
1:B:85:THR:HG23	1:B:88:PRO:CG	2.52	0.40
1:B:407:THR:O	1:B:407:THR:HG22	2.21	0.40
1:B:76:LEU:HD11	1:B:92:LEU:HD12	2.03	0.40
1:A:221:GLN:HE21	1:A:221:GLN:CA	2.34	0.40
1:B:315:SER:HB2	1:B:328:THR:CG2	2.52	0.40
1:B:356:PHE:HA	6:B:581:HOH:O	2.20	0.40
2:A:438:NAG:H3	3:A:440:MAN:O2	2.22	0.40
1:B:146:ARG:HH11	1:B:146:ARG:HG3	1.85	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:TYR:CD1	1:A:109:TYR:N	2.89	0.40
1:A:248:SER:O	1:A:249:GLN:HB2	2.21	0.40
1:A:280:ASN:ND2	1:A:393:PRO:CG	2.84	0.40
3:A:447:MAN:O4	3:A:448:MAN:H3	2.21	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	411/437 (94%)	361 (88%)	45 (11%)	5 (1%)	19	31
1	B	411/437 (94%)	371 (90%)	37 (9%)	3 (1%)	30	49
All	All	822/874 (94%)	732 (89%)	82 (10%)	8 (1%)	22	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	VAL
1	A	300	TYR
1	B	245	THR
1	A	214	GLN
1	A	272	TYR
1	B	295	VAL
1	B	110	ASN
1	A	110	ASN

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	341/358 (95%)	315 (92%)	26 (8%)	19	33
1	B	341/358 (95%)	315 (92%)	26 (8%)	19	33
All	All	682/716 (95%)	630 (92%)	52 (8%)	19	33

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	56	VAL
1	A	85	THR
1	A	92	LEU
1	A	93	LEU
1	A	96	VAL
1	A	104	ARG
1	A	139	GLU
1	A	146	ARG
1	A	172	GLU
1	A	187	ASN
1	A	201	THR
1	A	218	ARG
1	A	228	ILE
1	A	245	THR
1	A	265	ASN
1	A	268	ASN
1	A	290	THR
1	A	329	ARG
1	A	364	GLN
1	A	370	ASN
1	A	379	LEU
1	A	399	ASN
1	A	406	ASN
1	A	414	LEU
1	A	424	LEU
1	B	32	ARG
1	B	56	VAL
1	B	85	THR
1	B	92	LEU
1	B	93	LEU
1	B	95	ASP
1	B	104	ARG
1	B	163	LEU
1	B	172	GLU

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Mol	Chain	Res	Type
1	B	201	THR
1	B	227	LEU
1	B	228	ILE
1	B	248	SER
1	B	265	ASN
1	B	267	ASN
1	B	268	ASN
1	B	282	PRO
1	B	329	ARG
1	B	346	VAL
1	B	353	LEU
1	B	364	GLN
1	B	369	CYS
1	B	370	ASN
1	B	379	LEU
1	B	386	CYS
1	B	424	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	44	GLN
1	A	63	ASN
1	A	103	GLN
1	A	110	ASN
1	A	128	ASN
1	A	156	ASN
1	A	157	GLN
1	A	171	HIS
1	A	182	GLN
1	A	187	ASN
1	A	221	GLN
1	A	232	GLN
1	A	246	GLN
1	A	265	ASN
1	A	268	ASN
1	A	280	ASN
1	A	302	ASN
1	A	319	GLN
1	A	364	GLN
1	A	370	ASN

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	399	ASN
1	A	406	ASN
1	A	415	ASN
1	B	43	GLN
1	B	44	GLN
1	B	54	ASN
1	B	63	ASN
1	B	108	HIS
1	B	128	ASN
1	B	156	ASN
1	B	171	HIS
1	B	182	GLN
1	B	187	ASN
1	B	232	GLN
1	B	265	ASN
1	B	268	ASN
1	B	302	ASN
1	B	364	GLN
1	B	370	ASN
1	B	376	ASN
1	B	399	ASN
1	B	406	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 4 are monoatomic - leaving 34 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	438	-	15,15,15	0.35	0	21,21,21	1.04	1 (4%)
3	MAN	A	439	-	12,12,12	0.52	0	17,17,17	0.57	0
3	MAN	A	440	-	12,12,12	0.65	0	17,17,17	1.29	2 (11%)
3	MAN	A	441	-	12,12,12	0.51	0	17,17,17	1.09	2 (11%)
3	MAN	A	442	-	12,12,12	0.36	0	17,17,17	0.89	1 (5%)
3	MAN	A	443	-	12,12,12	0.56	0	17,17,17	1.06	2 (11%)
2	NAG	A	444	-	15,15,15	0.70	0	21,21,21	0.97	1 (4%)
3	MAN	A	445	-	12,12,12	0.48	0	17,17,17	0.57	0
4	NDG	A	446	-	15,15,15	0.74	0	21,21,21	1.34	2 (9%)
3	MAN	A	447	-	12,12,12	0.57	0	17,17,17	0.94	1 (5%)
3	MAN	A	448	-	12,12,12	0.52	0	17,17,17	0.79	0
4	NDG	A	449	-	15,15,15	0.51	0	21,21,21	0.94	2 (9%)
2	NAG	A	450	-	15,15,15	0.69	0	21,21,21	1.10	2 (9%)
3	MAN	A	451	-	12,12,12	0.40	0	17,17,17	0.66	0
3	MAN	A	452	-	12,12,12	0.42	0	17,17,17	0.66	0
3	MAN	A	453	-	12,12,12	0.66	0	17,17,17	0.83	0
3	MAN	A	454	-	12,12,12	0.50	0	17,17,17	0.58	0
2	NAG	B	538	-	15,15,15	0.58	0	21,21,21	1.25	3 (14%)
3	MAN	B	539	-	12,12,12	0.60	0	17,17,17	0.94	1 (5%)
3	MAN	B	540	-	12,12,12	0.32	0	17,17,17	0.59	0
3	MAN	B	541	-	12,12,12	0.59	0	17,17,17	0.95	1 (5%)
3	MAN	B	542	-	12,12,12	0.46	0	17,17,17	0.67	0
3	MAN	B	543	-	12,12,12	0.46	0	17,17,17	0.77	0
4	NDG	B	544	-	15,15,15	0.43	0	21,21,21	0.96	1 (4%)
3	MAN	B	545	-	12,12,12	0.65	0	17,17,17	0.45	0
2	NAG	B	546	-	15,15,15	0.73	0	21,21,21	0.98	1 (4%)
3	MAN	B	547	-	12,12,12	0.56	0	17,17,17	0.48	0
3	MAN	B	548	-	12,12,12	0.40	0	17,17,17	0.54	0
2	NAG	B	549	-	15,15,15	0.43	0	21,21,21	0.71	0
4	NDG	B	550	-	15,15,15	0.59	0	21,21,21	0.76	1 (4%)
3	MAN	B	551	-	12,12,12	0.55	0	17,17,17	0.61	0
3	MAN	B	552	-	12,12,12	0.67	0	17,17,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	B	553	-	12,12,12	0.49	0	17,17,17	0.67	0
3	MAN	B	554	-	12,12,12	0.60	0	17,17,17	0.96	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	438	-	-	0/6/26/26	0/1/1/1
3	MAN	A	439	-	1/1/5/5	0/2/22/22	0/1/1/1
3	MAN	A	440	-	-	0/2/22/22	0/1/1/1
3	MAN	A	441	-	-	0/2/22/22	0/1/1/1
3	MAN	A	442	-	1/1/5/5	0/2/22/22	0/1/1/1
3	MAN	A	443	-	-	0/2/22/22	0/1/1/1
2	NAG	A	444	-	-	0/6/26/26	0/1/1/1
3	MAN	A	445	-	-	0/2/22/22	0/1/1/1
4	NDG	A	446	-	-	0/6/26/26	0/1/1/1
3	MAN	A	447	-	1/1/5/5	0/2/22/22	0/1/1/1
3	MAN	A	448	-	-	0/2/22/22	0/1/1/1
4	NDG	A	449	-	-	0/6/26/26	0/1/1/1
2	NAG	A	450	-	-	0/6/26/26	0/1/1/1
3	MAN	A	451	-	1/1/5/5	0/2/22/22	0/1/1/1
3	MAN	A	452	-	-	0/2/22/22	1/1/1/1
3	MAN	A	453	-	-	0/2/22/22	0/1/1/1
3	MAN	A	454	-	1/1/5/5	0/2/22/22	0/1/1/1
2	NAG	B	538	-	-	0/6/26/26	0/1/1/1
3	MAN	B	539	-	-	0/2/22/22	0/1/1/1
3	MAN	B	540	-	-	0/2/22/22	0/1/1/1
3	MAN	B	541	-	-	0/2/22/22	0/1/1/1
3	MAN	B	542	-	-	0/2/22/22	0/1/1/1
3	MAN	B	543	-	1/1/5/5	0/2/22/22	0/1/1/1
4	NDG	B	544	-	-	0/6/26/26	0/1/1/1
3	MAN	B	545	-	-	0/2/22/22	1/1/1/1
2	NAG	B	546	-	-	0/6/26/26	0/1/1/1
3	MAN	B	547	-	1/1/5/5	0/2/22/22	0/1/1/1
3	MAN	B	548	-	1/1/5/5	0/2/22/22	0/1/1/1
2	NAG	B	549	-	-	0/6/26/26	0/1/1/1
4	NDG	B	550	-	-	0/6/26/26	0/1/1/1
3	MAN	B	551	-	1/1/5/5	0/2/22/22	0/1/1/1
3	MAN	B	552	-	-	0/2/22/22	0/1/1/1
3	MAN	B	553	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	B	554	-	1/1/5/5	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	446	NDG	C4-C3-C2	-4.32	104.31	110.44
3	A	440	MAN	C1-C2-C3	3.85	116.64	110.53
2	B	538	NAG	O5-C1-C2	2.99	112.64	109.61
2	A	450	NAG	O5-C1-C2	2.95	112.60	109.61
3	A	441	MAN	C4-C3-C2	-2.85	105.55	110.82
3	A	443	MAN	C3-C4-C5	2.80	115.21	110.20
2	B	546	NAG	O5-C1-C2	2.69	112.33	109.61
2	A	438	NAG	C4-C3-C2	2.66	114.22	110.44
4	B	544	NDG	C1-C2-C3	-2.64	106.81	110.59
3	A	440	MAN	O5-C1-C2	2.58	113.85	109.86
3	A	447	MAN	C4-C3-C2	-2.55	106.10	110.82
3	B	539	MAN	C3-C4-C5	-2.53	105.68	110.20
2	B	538	NAG	C4-C3-C2	-2.53	106.85	110.44
2	B	538	NAG	C6-C5-C4	-2.50	106.96	113.00
3	B	554	MAN	C1-C2-C3	2.50	114.50	110.53
3	A	443	MAN	C4-C3-C2	2.45	115.35	110.82
4	A	446	NDG	C3-C4-C5	-2.43	105.87	110.20
4	A	449	NDG	C1-C2-C3	-2.43	107.12	110.59
2	A	444	NAG	C1-C2-N2	-2.36	108.10	110.85
2	A	450	NAG	C1-C2-N2	-2.31	108.16	110.85
3	A	441	MAN	C3-C4-C5	-2.21	106.26	110.20
4	A	449	NDG	C4-C3-C2	-2.20	107.32	110.44
4	B	550	NDG	C1-C2-N2	-2.18	108.31	110.85
3	A	442	MAN	C3-C4-C5	2.18	114.09	110.20
3	B	541	MAN	C3-C4-C5	-2.08	106.49	110.20

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	554	MAN	C1
3	A	451	MAN	C1
3	A	447	MAN	C1
3	A	439	MAN	C1
3	B	548	MAN	C1
3	A	442	MAN	C1
3	A	454	MAN	C1

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Mol	Chain	Res	Type	Atom
3	B	543	MAN	C1
3	B	551	MAN	C1
3	B	547	MAN	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	452	MAN	C1-C2-C3-C4-C5-O5
3	B	545	MAN	C1-C2-C3-C4-C5-O5

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	413/437 (94%)	0.31	11 (2%) 52 55	22, 34, 48, 52	0
1	B	413/437 (94%)	0.35	6 (1%) 70 73	21, 34, 48, 55	0
All	All	826/874 (94%)	0.33	17 (2%) 62 64	21, 34, 48, 55	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	VAL	3.2
1	B	244	THR	2.8
1	B	292	ALA	2.8
1	B	140	LEU	2.6
1	A	194	ILE	2.4
1	A	195	ALA	2.3
1	A	437	ASN	2.2
1	A	292	ALA	2.2
1	B	387	SER	2.2
1	A	320	LEU	2.1
1	B	295	VAL	2.1
1	B	283	GLY	2.1
1	A	410	LEU	2.1
1	A	425	ARG	2.1
1	A	276	THR	2.1
1	A	47	ASN	2.0
1	A	199	GLN	2.0

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 ⓘ

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
3	MAN	A	439	12/12	0.29	8.36	52,53,54,56	0
4	NDG	A	446	15/15	0.29	5.03	55,56,59,59	0
4	NDG	A	449	15/15	0.32	4.55	45,48,51,51	0
2	NAG	A	438	15/15	0.33	3.77	56,56,58,59	0
2	NAG	B	549	15/15	0.35	3.43	43,49,51,53	0
2	NAG	B	538	15/15	0.32	3.26	55,57,61,63	0
3	MAN	A	452	12/12	0.29	2.89	50,53,55,55	0
2	NAG	B	546	15/15	0.28	2.83	50,55,60,60	0
3	MAN	B	539	12/12	0.27	1.93	52,53,54,55	0
3	MAN	A	441	12/12	0.23	1.08	54,57,58,59	0
3	MAN	A	453	12/12	0.23	1.07	39,41,42,42	0
4	NDG	B	550	15/15	0.27	1.04	53,55,56,56	0
3	MAN	A	443	12/12	0.23	0.95	51,51,52,53	0
2	NAG	A	444	15/15	0.18	0.80	38,43,46,48	0
3	MAN	B	543	12/12	0.24	0.63	50,50,52,52	0
3	MAN	B	553	12/12	0.23	0.56	37,40,43,43	0
3	MAN	B	548	12/12	0.29	0.38	55,56,58,60	0
3	MAN	B	552	12/12	0.27	0.34	49,53,54,54	0
2	NAG	A	450	15/15	0.23	0.05	55,55,56,56	0
4	NDG	B	544	15/15	0.19	-0.27	38,44,45,46	0
3	MAN	B	541	12/12	0.25	-0.28	56,57,59,60	0
5	HG	B	457	1/1	0.10	-1.45	69,69,69,69	1
5	HG	A	455	1/1	0.09	-1.77	61,61,61,61	1
5	HG	B	458	1/1	0.09	-3.00	86,86,86,86	1
5	HG	A	456	1/1	0.11	-3.26	71,71,71,71	0
3	MAN	A	440	12/12	0.32	-	54,55,58,59	0
3	MAN	A	454	12/12	0.26	-	48,50,53,54	0
3	MAN	B	554	12/12	0.35	-	50,53,54,55	0
3	MAN	B	540	12/12	0.34	-	54,55,58,58	0
3	MAN	A	448	12/12	0.17	-	53,54,56,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MAN	B	542	12/12	0.27	-	64,66,67,69	0
3	MAN	B	551	12/12	0.24	-	59,61,62,63	0
3	MAN	A	447	12/12	0.20	-	58,58,59,59	0
3	MAN	A	442	12/12	0.38	-	64,65,66,66	0
3	MAN	A	445	12/12	0.35	-	64,66,67,69	0
3	MAN	B	547	12/12	0.32	-	58,59,61,62	0
3	MAN	B	545	12/12	0.42	-	64,66,67,67	0
3	MAN	A	451	12/12	0.20	-	60,62,63,63	0

6.5 Other polymers

There are no such residues in this entry.