



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:42 AM GMT

PDB ID : 1M3Y
Title : The Structure of 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 : 2002-07-01
Resolution : 2.00 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>

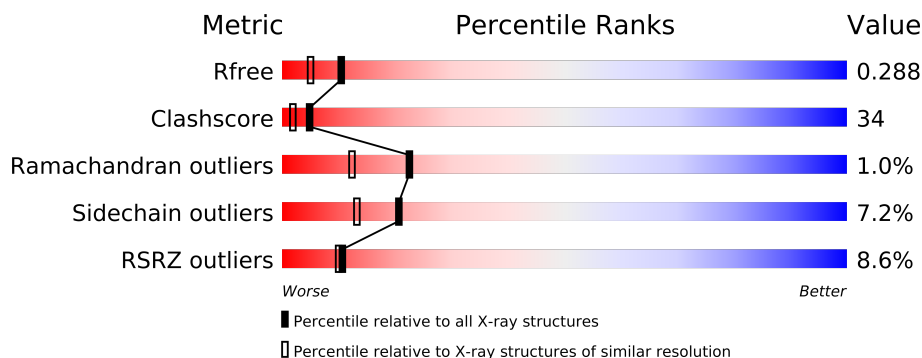
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	413	
1	B	413	
1	C	413	
1	D	413	

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	NDG	A	442	-	X
2	NDG	B	538	-	X
2	NDG	C	638	-	X
2	NDG	D	738	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	NDG	D	742	-	X
3	MAN	A	439	-	X
3	MAN	B	539	-	X
3	MAN	C	639	-	X
5	HG	C	644	-	X
5	HG	D	744	-	X

2 Entry composition i

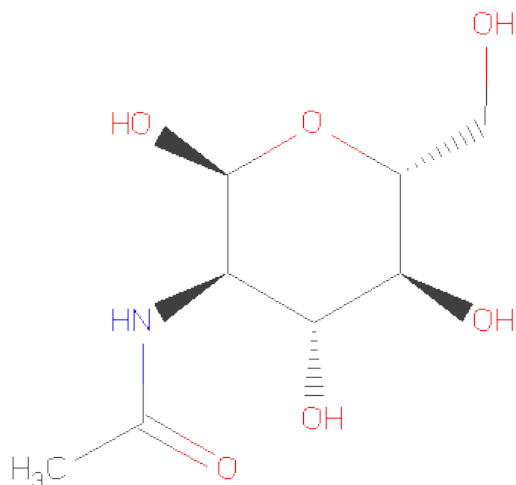
There are 6 unique types of molecules in this entry. The entry contains 13261 atoms, of which 0 are hydrogen and 0 are deuterium.

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 The Major capsid protein of PBCV-1, Vp54.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3231	2052	549	622	8			
1	B	413	Total	C	N	O	S	0	0	0
			3231	2052	549	622	8			
1	C	413	Total	C	N	O	S	0	0	0
			3231	2052	549	622	8			
1	D	413	Total	C	N	O	S	0	0	0
			3231	2052	549	622	8			

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



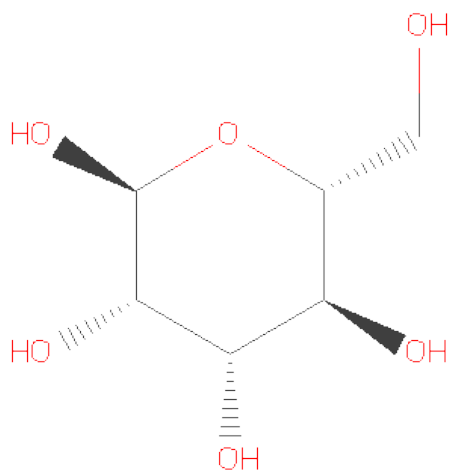
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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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		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		

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



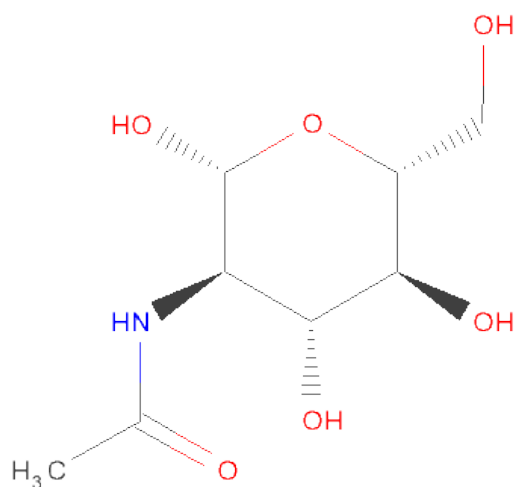
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total 2	Hg 2	0	0
5	C	2	Total 2	Hg 2	0	0

- Molecule 6 is water.

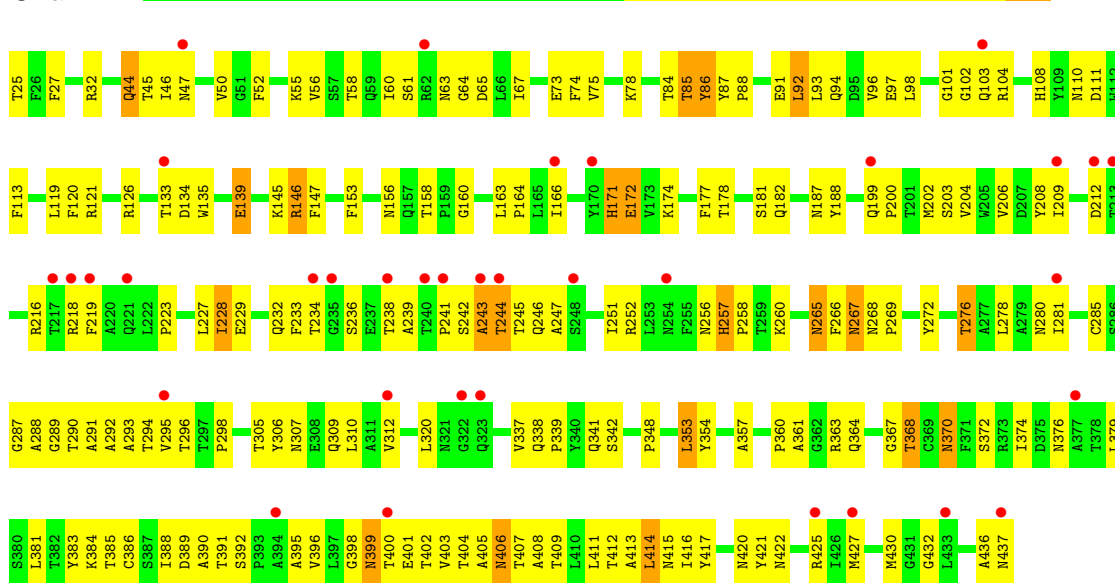
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total 24	O 24	0	0
6	B	9	Total 9	O 9	0	0
6	C	8	Total 8	O 8	0	0
6	D	12	Total 12	O 12	0	0

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 ($\text{RSRZ} > 2$). 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.

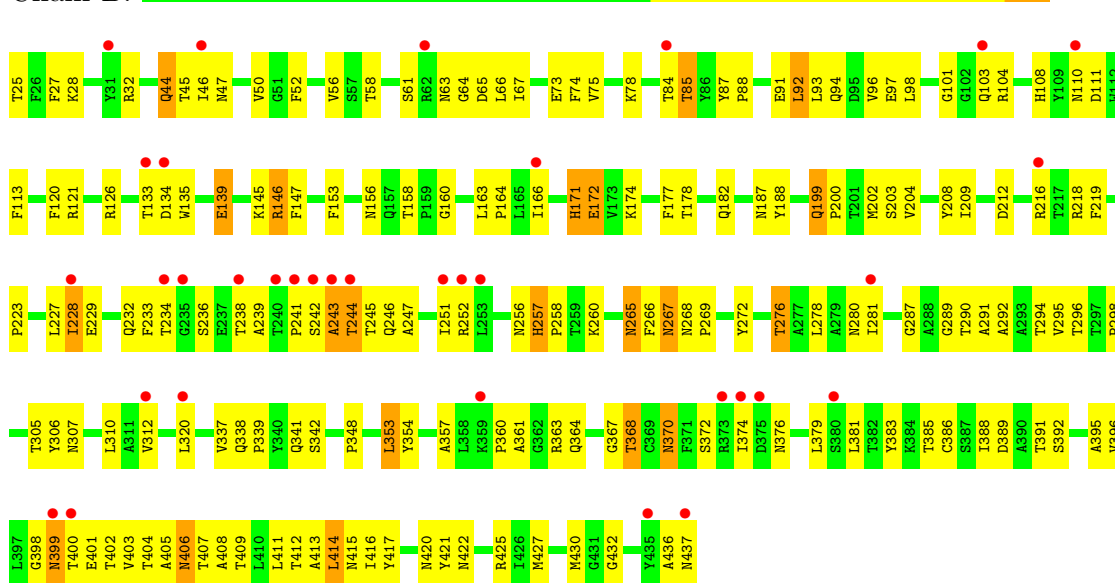
- Molecule 1: The Major capsid protein of PBCV-1, Vp54

Chain A:



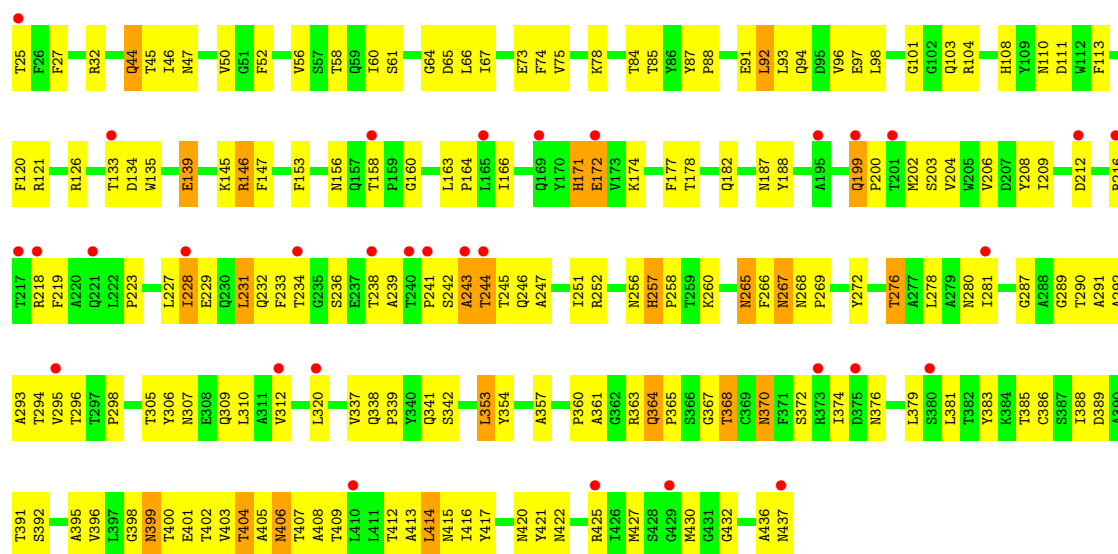
- Molecule 1: The Major capsid protein of PBCV-1, Vp54

Chain B:



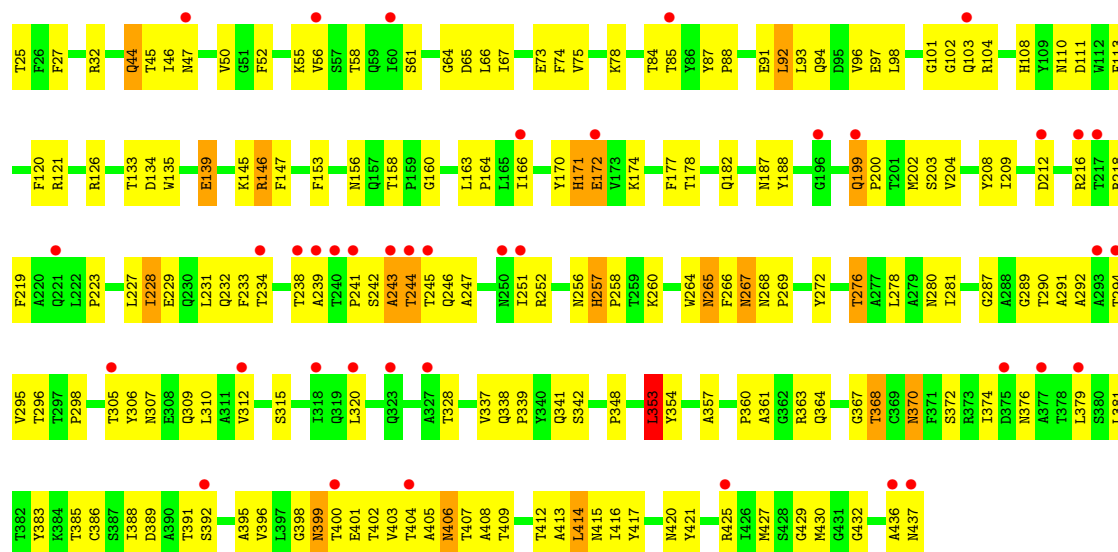
• Molecule 1: The Major capsid protein of PBCV-1, Vp54

Chain C: 



• Molecule 1: The Major capsid protein of PBCV-1, Vp54

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	188.79Å 188.79Å 188.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.43 – 2.00 84.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (84.43-2.00) 92.5 (84.43-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.342 , 0.352 0.274 , 0.288	Depositor DCC
R_{free} test set	4095 reflections (3.03%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 34.1	EDS
Estimated twinning fraction	0.278 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 146411 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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	0.44	3/3306 (0.1%)	0.68	4/4506 (0.1%)
1	B	0.40	0/3306	0.65	1/4506 (0.0%)
1	C	0.39	0/3306	0.64	1/4506 (0.0%)
1	D	0.39	0/3306	0.65	1/4506 (0.0%)
All	All	0.41	3/13224 (0.0%)	0.66	7/18024 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	LEU	CG-CD2	-7.86	1.22	1.51
1	A	86	TYR	CE1-CZ	6.26	1.46	1.38
1	A	86	TYR	CD1-CE1	-5.79	1.30	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	TYR	CG-CD1-CE1	-9.57	113.64	121.30
1	A	119	LEU	CB-CG-CD2	-7.96	97.46	111.00
1	C	353	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	86	TYR	CE1-CZ-CE2	-5.71	110.66	119.80
1	A	353	LEU	CA-CB-CG	5.66	128.31	115.30
1	D	353	LEU	CA-CB-CG	5.59	128.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	LEU	CA-CB-CG	5.51	127.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	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	3231	0	3128	221	0
1	B	3231	0	3128	208	0
1	C	3231	0	3128	204	0
1	D	3231	0	3128	220	0
2	A	30	0	30	22	0
2	B	30	0	30	18	0
2	C	30	0	30	22	0
2	D	30	0	30	24	0
3	A	24	0	24	10	0
3	B	24	0	24	11	0
3	C	24	0	24	9	0
3	D	24	0	24	11	0
4	A	15	0	15	15	0
4	B	15	0	15	14	0
4	C	15	0	15	14	0
4	D	15	0	15	16	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	1	0
6	A	24	0	0	4	0
6	B	9	0	0	1	0
6	C	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	12	0	0	1	0
All	All	13261	0	12788	887	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 34.

All (887) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:638:NDG:H4	3:C:639:MAN:O2	1.45	1.16
2:B:538:NDG:H4	3:B:539:MAN:O2	1.45	1.14
2:D:738:NDG:H4	3:D:739:MAN:O2	1.50	1.11
2:A:438:NDG:H4	3:A:439:MAN:O2	1.49	1.09
2:B:538:NDG:C4	3:B:539:MAN:O2	2.07	1.03
1:D:88:PRO:HD2	1:D:134:ASP:HB3	1.37	1.02
1:A:88:PRO:HD2	1:A:134:ASP:HB3	1.36	1.02
1:C:88:PRO:HD2	1:C:134:ASP:HB3	1.40	1.02
1:B:88:PRO:HD2	1:B:134:ASP:HB3	1.40	1.00
1:A:305:THR:HG22	1:A:307:ASN:H	1.26	0.99
2:A:438:NDG:C4	3:A:439:MAN:O2	2.12	0.98
1:D:305:THR:HG22	1:D:307:ASN:H	1.28	0.97
1:B:305:THR:HG22	1:B:307:ASN:H	1.27	0.96
2:D:738:NDG:C4	3:D:739:MAN:O2	2.12	0.96
1:A:290:THR:HG23	1:A:292:ALA:H	1.30	0.96
2:C:638:NDG:C4	3:C:639:MAN:O2	2.14	0.95
1:D:290:THR:HG23	1:D:292:ALA:H	1.30	0.94
1:C:305:THR:HG22	1:C:307:ASN:H	1.29	0.93
1:B:290:THR:HG23	1:B:292:ALA:H	1.33	0.93
1:A:406:ASN:O	2:A:442:NDG:H8C3	1.70	0.92
1:D:406:ASN:O	2:D:742:NDG:H8C3	1.70	0.92
1:C:406:ASN:O	2:C:642:NDG:H8C3	1.70	0.90
1:C:153:PHE:H	1:C:156:ASN:HD22	1.21	0.89
1:C:290:THR:HG23	1:C:292:ALA:H	1.33	0.89
1:D:153:PHE:H	1:D:156:ASN:HD22	1.20	0.89
1:A:104:ARG:HD3	1:D:102:GLY:HA3	1.53	0.88
1:D:25:THR:HG22	1:D:27:PHE:H	1.39	0.87
1:C:25:THR:HG22	1:C:27:PHE:H	1.41	0.85
1:B:406:ASN:O	2:B:542:NDG:H8C3	1.76	0.85
1:A:25:THR:HG22	1:A:27:PHE:H	1.41	0.85
1:C:388:ILE:HA	4:C:640:NAG:O7	1.76	0.84
1:B:398:GLY:O	4:B:540:NAG:H62	1.75	0.84
1:A:153:PHE:H	1:A:156:ASN:HD22	1.23	0.84
1:C:289:GLY:HA2	2:C:638:NDG:O7	1.78	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:398:GLY:O	4:C:640:NAG:H62	1.78	0.84
1:B:25:THR:HG22	1:B:27:PHE:H	1.43	0.84
1:B:135:TRP:CD1	1:B:139:GLU:HG3	2.13	0.83
1:A:135:TRP:CD1	1:A:139:GLU:HG3	2.13	0.83
1:C:135:TRP:CD1	1:C:139:GLU:HG3	2.12	0.83
1:D:88:PRO:HD2	1:D:134:ASP:CB	2.08	0.83
1:B:153:PHE:H	1:B:156:ASN:HD22	1.23	0.83
1:D:135:TRP:CD1	1:D:139:GLU:HG3	2.13	0.83
1:D:216:ARG:HH11	1:D:216:ARG:HG2	1.42	0.82
1:D:388:ILE:HA	4:D:740:NAG:O7	1.81	0.81
1:D:398:GLY:O	4:D:740:NAG:H62	1.79	0.81
1:B:216:ARG:HH11	1:B:216:ARG:HG2	1.45	0.81
1:C:216:ARG:HH11	1:C:216:ARG:HG2	1.45	0.81
1:A:388:ILE:HA	4:A:440:NAG:O7	1.80	0.81
1:A:88:PRO:HD2	1:A:134:ASP:CB	2.10	0.81
1:C:399:ASN:HD21	4:C:640:NAG:C1	1.93	0.81
1:A:399:ASN:HD21	4:A:440:NAG:C1	1.94	0.81
1:B:388:ILE:HA	4:B:540:NAG:O7	1.82	0.80
1:A:398:GLY:O	4:A:440:NAG:H62	1.81	0.80
1:A:289:GLY:HA2	2:A:438:NDG:O7	1.81	0.79
1:B:88:PRO:HD2	1:B:134:ASP:CB	2.13	0.79
1:D:287:GLY:O	1:D:290:THR:HG22	1.81	0.79
1:B:287:GLY:O	1:B:290:THR:HG22	1.82	0.79
1:A:93:LEU:HD21	1:A:177:PHE:HD2	1.48	0.78
1:C:146:ARG:HG2	1:C:146:ARG:HH11	1.46	0.78
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.46	0.78
1:D:399:ASN:HD21	4:D:740:NAG:C1	1.96	0.78
1:B:399:ASN:HD21	4:B:540:NAG:C1	1.95	0.78
1:D:289:GLY:HA2	2:D:738:NDG:O7	1.83	0.78
1:C:88:PRO:HD2	1:C:134:ASP:CB	2.12	0.78
1:B:289:GLY:HA2	2:B:538:NDG:O7	1.83	0.78
1:A:287:GLY:O	1:A:290:THR:HG22	1.84	0.78
1:D:146:ARG:HG2	1:D:146:ARG:HH11	1.49	0.77
1:D:93:LEU:HD21	1:D:177:PHE:HD2	1.47	0.77
1:C:93:LEU:HD21	1:C:177:PHE:HD2	1.48	0.77
1:D:280:ASN:HD21	2:D:738:NDG:C5	1.98	0.77
1:B:88:PRO:HG3	6:B:549:HOH:O	1.84	0.77
1:B:46:ILE:HG23	1:B:56:VAL:HG21	1.67	0.77
1:C:280:ASN:HD21	2:C:638:NDG:C5	1.98	0.76
1:C:312:VAL:HG12	1:C:408:ALA:HB1	1.68	0.76
1:C:287:GLY:O	1:C:290:THR:HG22	1.85	0.76
1:B:93:LEU:HD21	1:B:177:PHE:HD2	1.51	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:46:ILE:HG23	1:C:56:VAL:HG21	1.67	0.75
1:D:238:THR:HB	1:D:412:THR:HA	1.66	0.75
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.50	0.75
1:D:241:PRO:HB2	1:D:245:THR:O	1.86	0.75
1:A:312:VAL:HG12	1:A:408:ALA:HB1	1.68	0.75
1:B:238:THR:HB	1:B:412:THR:HA	1.68	0.75
1:D:46:ILE:HG23	1:D:56:VAL:HG21	1.67	0.74
1:A:241:PRO:HB2	1:A:245:THR:O	1.86	0.74
2:D:738:NDG:C4	3:D:739:MAN:HO2	2.01	0.74
1:C:241:PRO:HB2	1:C:245:THR:O	1.88	0.74
1:D:97:GLU:OE2	1:D:104:ARG:HD2	1.88	0.74
1:D:312:VAL:HG12	1:D:408:ALA:HB1	1.70	0.74
2:C:638:NDG:C4	3:C:639:MAN:HO2	2.00	0.74
1:C:361:ALA:HB3	6:C:647:HOH:O	1.88	0.74
1:A:46:ILE:HG23	1:A:56:VAL:HG21	1.69	0.73
1:A:291:ALA:HA	3:A:439:MAN:H1	1.70	0.73
2:A:438:NDG:H4	3:A:439:MAN:C2	2.19	0.73
1:B:146:ARG:HH11	1:B:146:ARG:HG2	1.50	0.73
1:B:312:VAL:HG12	1:B:408:ALA:HB1	1.70	0.73
1:A:238:THR:HB	1:A:412:THR:HA	1.68	0.73
1:C:238:THR:HB	1:C:412:THR:HA	1.70	0.73
1:C:406:ASN:ND2	2:C:642:NDG:H1	2.03	0.73
1:B:406:ASN:ND2	2:B:542:NDG:H1	2.04	0.72
1:A:212:ASP:O	1:A:216:ARG:HG3	1.88	0.72
1:D:88:PRO:CD	1:D:134:ASP:HB3	2.17	0.72
1:D:406:ASN:ND2	2:D:742:NDG:H1	2.04	0.72
1:B:97:GLU:OE2	1:B:104:ARG:HD2	1.88	0.72
2:C:638:NDG:H4	3:C:639:MAN:C2	2.19	0.72
2:D:738:NDG:H4	3:D:739:MAN:C2	2.19	0.71
1:C:291:ALA:HA	3:C:639:MAN:H1	1.73	0.71
1:B:291:ALA:HA	3:B:539:MAN:H1	1.72	0.71
1:A:241:PRO:HD3	1:A:247:ALA:HB3	1.72	0.71
1:B:212:ASP:O	1:B:216:ARG:HG3	1.90	0.71
1:C:88:PRO:CD	1:C:134:ASP:HB3	2.19	0.71
1:D:78:LYS:CD	1:D:139:GLU:HB2	2.20	0.71
1:D:280:ASN:HD21	2:D:738:NDG:H6C2	1.57	0.70
1:A:406:ASN:ND2	2:A:442:NDG:H1	2.07	0.70
1:B:241:PRO:HD3	1:B:247:ALA:HB3	1.73	0.70
2:B:538:NDG:H4	3:B:539:MAN:C2	2.22	0.70
1:B:241:PRO:HB2	1:B:245:THR:O	1.92	0.70
1:A:97:GLU:OE2	1:A:104:ARG:HD2	1.92	0.70
1:C:46:ILE:HG23	1:C:56:VAL:CG2	2.22	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:ASN:HD21	2:A:438:NDG:C5	2.04	0.70
1:A:88:PRO:CD	1:A:134:ASP:HB3	2.17	0.69
1:C:212:ASP:O	1:C:216:ARG:HG3	1.91	0.69
1:D:46:ILE:HG23	1:D:56:VAL:CG2	2.22	0.69
1:D:232:GLN:HE22	1:D:256:ASN:H	1.41	0.69
1:C:241:PRO:HD3	1:C:247:ALA:HB3	1.75	0.69
1:D:212:ASP:O	1:D:216:ARG:HG3	1.93	0.69
1:D:291:ALA:HA	3:D:739:MAN:H1	1.74	0.69
1:A:312:VAL:CG1	1:A:408:ALA:HB1	2.23	0.69
1:C:280:ASN:HD21	2:C:638:NDG:C6	2.06	0.68
1:A:243:ALA:O	1:A:245:THR:N	2.27	0.68
1:A:404:THR:HG22	1:A:405:ALA:H	1.59	0.68
1:D:280:ASN:HD21	2:D:738:NDG:C6	2.06	0.68
1:A:47:ASN:HD21	1:D:55:LYS:HE2	1.56	0.68
1:B:46:ILE:HG23	1:B:56:VAL:CG2	2.22	0.68
1:D:265:ASN:HD21	1:D:415:ASN:HD22	1.42	0.68
1:C:243:ALA:O	1:C:245:THR:N	2.27	0.68
1:C:78:LYS:CD	1:C:139:GLU:HB2	2.24	0.68
1:A:46:ILE:HG23	1:A:56:VAL:CG2	2.24	0.67
1:D:158:THR:HG22	1:D:160:GLY:H	1.59	0.67
1:A:280:ASN:HD21	2:A:438:NDG:H6C2	1.60	0.67
1:A:232:GLN:HE22	1:A:256:ASN:H	1.41	0.67
1:D:312:VAL:CG1	1:D:408:ALA:HB1	2.25	0.67
1:C:97:GLU:OE2	1:C:104:ARG:HD2	1.94	0.67
1:C:370:ASN:HD21	1:C:372:SER:HB2	1.60	0.67
1:C:242:SER:O	1:C:243:ALA:HB2	1.94	0.67
1:D:258:PRO:HB3	1:D:368:THR:HG21	1.75	0.67
1:A:406:ASN:CG	2:A:442:NDG:H1	2.16	0.66
1:C:312:VAL:CG1	1:C:408:ALA:HB1	2.24	0.66
1:B:88:PRO:CD	1:B:134:ASP:HB3	2.19	0.66
1:B:243:ALA:O	1:B:245:THR:N	2.28	0.66
1:C:232:GLN:HE22	1:C:256:ASN:H	1.43	0.66
1:A:280:ASN:HD21	2:A:438:NDG:C6	2.09	0.66
1:B:87:TYR:HD2	1:B:133:THR:HG21	1.61	0.66
1:D:78:LYS:HD2	1:D:139:GLU:HB2	1.75	0.66
1:D:241:PRO:HD3	1:D:247:ALA:HB3	1.78	0.66
1:A:242:SER:O	1:A:243:ALA:HB2	1.95	0.66
1:A:258:PRO:HB3	1:A:368:THR:HG21	1.77	0.66
1:C:258:PRO:HB3	1:C:368:THR:HG21	1.77	0.66
1:C:44:GLN:NE2	1:C:61:SER:H	1.94	0.66
1:C:87:TYR:N	1:C:88:PRO:HD3	2.11	0.65
1:A:78:LYS:CD	1:A:139:GLU:HB2	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:44:GLN:NE2	1:D:61:SER:H	1.94	0.65
1:B:280:ASN:HD21	2:B:538:NDG:H6C2	1.61	0.65
1:A:52:PHE:CE2	1:A:200:PRO:HD3	2.31	0.65
1:B:312:VAL:CG1	1:B:408:ALA:HB1	2.27	0.65
1:B:258:PRO:HB3	1:B:368:THR:HG21	1.78	0.65
1:C:280:ASN:ND2	2:C:638:NDG:C5	2.60	0.65
1:D:87:TYR:N	1:D:88:PRO:HD3	2.12	0.65
1:A:172:GLU:OE1	1:A:174:LYS:HD2	1.97	0.65
1:B:406:ASN:CG	2:B:542:NDG:H1	2.17	0.64
1:B:232:GLN:HE22	1:B:256:ASN:H	1.43	0.64
1:C:404:THR:HG22	1:C:405:ALA:H	1.62	0.64
1:D:280:ASN:ND2	2:D:738:NDG:C5	2.59	0.64
1:B:78:LYS:CD	1:B:139:GLU:HB2	2.27	0.64
1:C:280:ASN:HD21	2:C:638:NDG:H6C2	1.62	0.64
1:A:158:THR:HG22	1:A:160:GLY:H	1.63	0.64
1:B:158:THR:OG1	1:B:363:ARG:HG3	1.98	0.64
1:A:163:LEU:HD22	1:A:164:PRO:HD2	1.80	0.64
1:B:44:GLN:NE2	1:B:61:SER:H	1.94	0.64
1:D:404:THR:HG22	1:D:405:ALA:H	1.63	0.64
1:A:87:TYR:N	1:A:88:PRO:HD3	2.12	0.64
1:A:388:ILE:HD11	1:A:403:VAL:HG23	1.79	0.64
1:D:242:SER:O	1:D:243:ALA:HB2	1.97	0.64
1:B:370:ASN:ND2	1:B:372:SER:H	1.96	0.64
1:B:400:THR:HG22	1:B:402:THR:H	1.62	0.64
1:C:52:PHE:CE2	1:C:200:PRO:HD3	2.33	0.64
1:D:163:LEU:HD22	1:D:164:PRO:HD2	1.80	0.64
1:D:400:THR:HG22	1:D:402:THR:H	1.62	0.63
1:C:241:PRO:HG3	1:C:246:GLN:HA	1.80	0.63
1:D:172:GLU:OE1	1:D:174:LYS:HD2	1.98	0.63
1:B:87:TYR:N	1:B:88:PRO:HD3	2.13	0.63
1:A:370:ASN:HD21	1:A:372:SER:HB2	1.63	0.63
1:D:87:TYR:HA	1:D:133:THR:HG22	1.80	0.63
1:C:172:GLU:OE1	1:C:174:LYS:HD2	1.99	0.63
1:C:163:LEU:HD22	1:C:164:PRO:HD2	1.80	0.63
1:B:370:ASN:HD21	1:B:372:SER:HB2	1.61	0.63
1:A:44:GLN:NE2	1:A:61:SER:H	1.96	0.63
1:D:134:ASP:HA	1:D:147:PHE:CE2	2.34	0.63
1:C:388:ILE:HD11	1:C:403:VAL:HG23	1.81	0.63
1:B:158:THR:HG22	1:B:160:GLY:H	1.64	0.62
1:A:400:THR:HG22	1:A:402:THR:H	1.62	0.62
1:D:388:ILE:HD11	1:D:403:VAL:HG23	1.81	0.62
1:C:93:LEU:HD22	1:C:96:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:295:VAL:HG12	1:C:295:VAL:O	1.99	0.62
1:B:404:THR:HG22	1:B:405:ALA:H	1.63	0.62
1:C:158:THR:HG22	1:C:160:GLY:H	1.64	0.62
1:C:78:LYS:HD2	1:C:139:GLU:HB2	1.82	0.62
1:A:241:PRO:HG3	1:A:246:GLN:HA	1.81	0.62
1:A:134:ASP:HA	1:A:147:PHE:CE2	2.35	0.62
1:B:134:ASP:HA	1:B:147:PHE:CE2	2.35	0.62
1:B:52:PHE:CE2	1:B:200:PRO:HD3	2.35	0.62
1:C:400:THR:HG22	1:C:402:THR:H	1.63	0.62
1:C:406:ASN:CG	2:C:642:NDG:H1	2.20	0.62
1:A:78:LYS:HD2	1:A:139:GLU:HB2	1.82	0.62
1:A:93:LEU:HD22	1:A:96:VAL:HG22	1.82	0.62
1:D:241:PRO:HG3	1:D:246:GLN:HA	1.81	0.61
1:A:265:ASN:HD21	1:A:415:ASN:HD22	1.48	0.61
1:B:87:TYR:HA	1:B:133:THR:HG22	1.81	0.61
1:B:242:SER:O	1:B:243:ALA:HB2	1.99	0.61
1:B:163:LEU:HD22	1:B:164:PRO:HD2	1.81	0.61
1:D:280:ASN:ND2	2:D:738:NDG:H6C2	2.16	0.61
1:B:243:ALA:C	1:B:245:THR:H	2.04	0.61
1:C:87:TYR:HD2	1:C:133:THR:HG21	1.64	0.61
1:A:102:GLY:HA3	1:D:104:ARG:HD3	1.82	0.61
1:A:243:ALA:C	1:A:245:THR:H	2.03	0.61
1:C:158:THR:OG1	1:C:363:ARG:HG3	2.00	0.61
1:D:45:THR:O	1:D:58:THR:HG23	2.01	0.61
1:B:280:ASN:HD21	2:B:538:NDG:C5	2.13	0.61
1:D:243:ALA:O	1:D:245:THR:N	2.34	0.61
1:C:243:ALA:C	1:C:245:THR:H	2.02	0.61
1:B:241:PRO:HG3	1:B:246:GLN:HA	1.82	0.61
1:D:370:ASN:HD21	1:D:372:SER:HB2	1.65	0.61
1:C:87:TYR:HA	1:C:133:THR:HG22	1.81	0.61
1:D:135:TRP:HB3	1:D:139:GLU:CG	2.30	0.61
1:D:93:LEU:HD22	1:D:96:VAL:HG22	1.83	0.60
1:A:338:GLN:HB2	1:A:339:PRO:HD3	1.83	0.60
1:D:87:TYR:HD2	1:D:133:THR:HG21	1.66	0.60
1:A:87:TYR:HA	1:A:133:THR:HG22	1.82	0.60
1:C:135:TRP:HB3	1:C:139:GLU:CG	2.30	0.60
1:B:216:ARG:CG	1:B:216:ARG:HH11	2.14	0.60
1:D:158:THR:OG1	1:D:363:ARG:HG3	2.01	0.60
1:C:370:ASN:ND2	1:C:372:SER:H	1.99	0.60
1:D:295:VAL:O	1:D:295:VAL:HG12	2.01	0.60
1:D:406:ASN:CG	2:D:742:NDG:H1	2.22	0.60
1:B:135:TRP:HB3	1:B:139:GLU:CG	2.31	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:93:LEU:HD22	1:B:96:VAL:HG22	1.81	0.60
1:B:280:ASN:HD21	2:B:538:NDG:C6	2.14	0.60
1:B:388:ILE:HD11	1:B:403:VAL:HG23	1.83	0.60
1:B:78:LYS:HD2	1:B:139:GLU:HB2	1.82	0.60
1:A:370:ASN:ND2	1:A:372:SER:H	2.00	0.60
1:B:172:GLU:OE1	1:B:174:LYS:HD2	2.00	0.60
1:D:243:ALA:C	1:D:245:THR:H	2.04	0.59
1:B:370:ASN:HD22	1:B:372:SER:H	1.50	0.59
1:A:295:VAL:HG12	1:A:295:VAL:O	2.01	0.59
1:A:280:ASN:ND2	2:A:438:NDG:H6C2	2.17	0.59
1:C:216:ARG:HH11	1:C:216:ARG:CG	2.14	0.59
1:A:135:TRP:HB3	1:A:139:GLU:CG	2.32	0.59
1:A:280:ASN:ND2	2:A:438:NDG:C5	2.65	0.59
1:B:265:ASN:HD21	1:B:415:ASN:HD22	1.49	0.59
1:D:216:ARG:HH11	1:D:216:ARG:CG	2.12	0.59
1:C:406:ASN:CG	2:C:642:NDG:H1L	2.05	0.59
1:B:338:GLN:HB2	1:B:339:PRO:HD3	1.85	0.59
1:D:52:PHE:CE2	1:D:200:PRO:HD3	2.38	0.59
1:B:94:GLN:HB3	1:B:178:THR:O	2.03	0.59
1:D:395:ALA:CB	4:D:740:NAG:H82	2.33	0.58
1:A:216:ARG:CG	1:A:216:ARG:HH11	2.16	0.58
1:D:238:THR:HG1	1:D:266:PHE:HD2	1.51	0.58
1:C:389:ASP:HB3	4:C:640:NAG:H81	1.86	0.58
1:C:293:ALA:HB3	2:C:638:NDG:O6	2.04	0.58
1:A:305:THR:HG22	1:A:306:TYR:N	2.19	0.58
1:C:395:ALA:CB	4:C:640:NAG:H82	2.34	0.58
1:A:158:THR:OG1	1:A:363:ARG:HG3	2.03	0.58
1:A:395:ALA:CB	4:A:440:NAG:H82	2.33	0.58
1:A:73:GLU:HB2	1:A:203:SER:HB3	1.85	0.58
1:D:171:HIS:CE1	1:D:430:MET:HB2	2.39	0.58
1:D:88:PRO:HG3	6:D:749:HOH:O	2.03	0.58
1:C:265:ASN:HD21	1:C:415:ASN:HD22	1.52	0.58
1:A:389:ASP:HB3	4:A:440:NAG:H81	1.84	0.58
1:D:46:ILE:CG2	1:D:56:VAL:HG21	2.34	0.58
1:A:174:LYS:HB3	1:A:174:LYS:NZ	2.19	0.58
1:C:338:GLN:HB2	1:C:339:PRO:HD3	1.84	0.58
4:C:640:NAG:H3	3:C:641:MAN:C1	2.34	0.57
1:D:64:GLY:HA3	1:D:208:TYR:HB3	1.86	0.57
1:D:93:LEU:HD21	1:D:177:PHE:CD2	2.36	0.57
1:C:370:ASN:HD22	1:C:372:SER:H	1.52	0.57
1:D:370:ASN:ND2	1:D:372:SER:H	2.02	0.57
1:B:295:VAL:O	1:B:295:VAL:HG12	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:146:ARG:HG2	1:D:146:ARG:NH1	2.19	0.57
1:C:238:THR:HG1	1:C:266:PHE:HD2	1.50	0.57
1:D:338:GLN:HB2	1:D:339:PRO:HD3	1.87	0.57
1:A:121:ARG:HG2	1:A:126:ARG:HA	1.86	0.57
1:C:134:ASP:HA	1:C:147:PHE:CE2	2.40	0.57
1:C:46:ILE:CG2	1:C:56:VAL:HG21	2.34	0.57
1:C:280:ASN:ND2	2:C:638:NDG:H6C2	2.19	0.57
1:A:45:THR:O	1:A:58:THR:HG23	2.05	0.57
1:C:94:GLN:HB3	1:C:178:THR:O	2.05	0.57
1:A:87:TYR:HD2	1:A:133:THR:HG21	1.69	0.57
1:B:389:ASP:HB3	4:B:540:NAG:H81	1.87	0.57
1:B:395:ALA:CB	4:B:540:NAG:H82	2.34	0.57
1:A:370:ASN:HD22	1:A:372:SER:H	1.51	0.57
1:B:174:LYS:NZ	1:B:174:LYS:HB3	2.19	0.57
1:D:386:CYS:SG	1:D:408:ALA:HB3	2.45	0.57
4:B:540:NAG:H3	3:B:541:MAN:C1	2.35	0.56
1:B:146:ARG:HG2	1:B:146:ARG:NH1	2.19	0.56
1:A:238:THR:HG1	1:A:266:PHE:HD2	1.53	0.56
1:D:305:THR:HG22	1:D:306:TYR:H	1.70	0.56
1:D:395:ALA:O	1:D:399:ASN:ND2	2.37	0.56
1:B:65:ASP:HA	1:B:166:ILE:HG23	1.87	0.56
1:A:93:LEU:HD21	1:A:177:PHE:CD2	2.36	0.56
4:A:440:NAG:H3	3:A:441:MAN:C1	2.36	0.56
1:D:94:GLN:HB3	1:D:178:THR:O	2.06	0.56
2:B:538:NDG:O4	3:B:539:MAN:O2	2.22	0.56
1:B:50:VAL:HG22	1:B:202:MET:CE	2.36	0.56
4:D:740:NAG:H3	3:D:741:MAN:C1	2.35	0.56
1:D:121:ARG:HG2	1:D:126:ARG:HA	1.87	0.56
1:C:174:LYS:NZ	1:C:174:LYS:HB3	2.20	0.56
1:D:209:ILE:N	1:D:209:ILE:HD12	2.21	0.56
1:A:305:THR:HG22	1:A:306:TYR:H	1.71	0.56
1:A:146:ARG:NH1	1:A:146:ARG:HG2	2.20	0.56
1:B:46:ILE:CG2	1:B:56:VAL:HG21	2.35	0.56
1:B:209:ILE:HD12	1:B:209:ILE:N	2.21	0.56
1:C:171:HIS:CE1	1:C:430:MET:HB2	2.41	0.56
1:A:171:HIS:CE1	1:A:430:MET:HB2	2.41	0.55
1:C:276:THR:HG23	1:C:310:LEU:HB3	1.87	0.55
1:D:305:THR:HG22	1:D:306:TYR:N	2.21	0.55
1:B:305:THR:HG22	1:B:306:TYR:N	2.20	0.55
1:C:45:THR:O	1:C:58:THR:HG23	2.05	0.55
1:B:45:THR:O	1:B:58:THR:HG23	2.06	0.55
1:B:251:ILE:HD12	1:B:251:ILE:N	2.20	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:251:ILE:N	1:C:251:ILE:HD12	2.22	0.55
1:B:121:ARG:HG2	1:B:126:ARG:HA	1.89	0.55
1:C:280:ASN:HB2	1:C:391:THR:HA	1.89	0.55
1:B:406:ASN:OD1	2:B:542:NDG:O1L	2.25	0.55
1:D:135:TRP:CG	1:D:139:GLU:HG3	2.42	0.55
1:C:386:CYS:SG	1:C:408:ALA:HB3	2.47	0.55
1:B:64:GLY:HA3	1:B:208:TYR:HB3	1.89	0.55
1:D:174:LYS:HB3	1:D:174:LYS:NZ	2.22	0.55
1:A:199:GLN:H	1:A:199:GLN:CD	2.10	0.55
1:B:386:CYS:SG	1:B:408:ALA:HB3	2.46	0.55
1:C:209:ILE:N	1:C:209:ILE:HD12	2.21	0.55
1:B:305:THR:HG22	1:B:306:TYR:H	1.71	0.54
1:A:395:ALA:O	1:A:399:ASN:ND2	2.40	0.54
1:B:93:LEU:HD21	1:B:177:PHE:CD2	2.39	0.54
1:D:73:GLU:HB2	1:D:203:SER:HB3	1.88	0.54
1:D:389:ASP:HB3	4:D:740:NAG:H81	1.89	0.54
1:B:280:ASN:HB2	1:B:391:THR:HA	1.89	0.54
1:B:238:THR:HG1	1:B:266:PHE:HD2	1.55	0.54
1:D:256:ASN:ND2	1:D:437:ASN:HB3	2.22	0.54
1:C:199:GLN:H	1:C:199:GLN:CD	2.10	0.54
1:B:280:ASN:ND2	2:B:538:NDG:H6C2	2.22	0.54
1:D:65:ASP:HA	1:D:166:ILE:HG23	1.88	0.54
1:D:50:VAL:HG22	1:D:202:MET:CE	2.37	0.54
1:C:400:THR:CG2	1:C:401:GLU:N	2.71	0.54
1:C:111:ASP:HB3	1:C:417:TYR:OH	2.07	0.54
1:C:73:GLU:HB2	1:C:203:SER:HB3	1.88	0.54
1:D:199:GLN:H	1:D:199:GLN:CD	2.10	0.54
1:C:146:ARG:HG2	1:C:146:ARG:NH1	2.16	0.54
1:B:199:GLN:H	1:B:199:GLN:CD	2.10	0.54
1:A:46:ILE:CG2	1:A:56:VAL:HG21	2.36	0.54
1:D:56:VAL:HG11	1:D:202:MET:CE	2.38	0.54
1:A:294:THR:HG22	1:A:296:THR:H	1.73	0.54
1:A:251:ILE:N	1:A:251:ILE:HD12	2.23	0.54
1:B:73:GLU:HB2	1:B:203:SER:HB3	1.89	0.54
1:D:294:THR:HG22	1:D:296:THR:H	1.73	0.54
1:A:278:LEU:HD21	1:A:298:PRO:HB3	1.89	0.53
1:B:171:HIS:CE1	1:B:430:MET:HB2	2.43	0.53
1:C:218:ARG:NH1	1:C:218:ARG:HB3	2.23	0.53
1:D:280:ASN:HB2	1:D:391:THR:HA	1.89	0.53
1:D:216:ARG:HG2	1:D:216:ARG:NH1	2.19	0.53
1:C:65:ASP:HA	1:C:166:ILE:HG23	1.89	0.53
1:A:64:GLY:HA3	1:A:208:TYR:HB3	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:440:NAG:O3	3:A:441:MAN:O5	2.26	0.53
1:A:46:ILE:HD13	1:A:202:MET:HE2	1.90	0.53
1:D:370:ASN:HD22	1:D:372:SER:H	1.56	0.53
1:C:395:ALA:O	1:C:399:ASN:ND2	2.41	0.53
1:A:50:VAL:HG22	1:A:202:MET:CE	2.39	0.53
1:A:65:ASP:HA	1:A:166:ILE:HG23	1.89	0.53
1:A:94:GLN:HB3	1:A:178:THR:O	2.08	0.53
1:A:320:LEU:HD22	1:A:374:ILE:HD13	1.89	0.53
1:A:280:ASN:HB2	1:A:391:THR:HA	1.91	0.53
1:B:353:LEU:HD22	1:B:354:TYR:N	2.23	0.53
1:D:74:PHE:CE2	1:D:92:LEU:HD13	2.43	0.53
1:B:276:THR:HG23	1:B:310:LEU:HB3	1.89	0.53
1:A:276:THR:HG23	1:A:310:LEU:HB3	1.91	0.53
1:A:135:TRP:HB3	1:A:139:GLU:HG2	1.90	0.53
1:C:50:VAL:HG22	1:C:202:MET:CE	2.39	0.53
1:A:244:THR:O	1:A:244:THR:HG22	2.09	0.53
1:C:305:THR:HG22	1:C:306:TYR:N	2.23	0.53
1:C:121:ARG:HG2	1:C:126:ARG:HA	1.90	0.53
1:B:67:ILE:HD11	1:B:163:LEU:HD12	1.90	0.53
1:D:406:ASN:CG	2:D:742:NDG:H1L	2.11	0.52
1:B:294:THR:HG22	1:B:296:THR:H	1.73	0.52
1:B:135:TRP:HB3	1:B:139:GLU:HG2	1.91	0.52
1:B:135:TRP:CG	1:B:139:GLU:HG3	2.43	0.52
1:C:400:THR:HG22	1:C:401:GLU:N	2.24	0.52
1:D:406:ASN:C	2:D:742:NDG:H8C3	2.29	0.52
1:A:395:ALA:HB1	4:A:440:NAG:H82	1.91	0.52
1:C:135:TRP:CG	1:C:139:GLU:HG3	2.43	0.52
1:C:146:ARG:HH11	1:C:146:ARG:CG	2.20	0.52
1:C:91:GLU:HA	1:C:110:ASN:OD1	2.09	0.52
1:B:320:LEU:HD22	1:B:374:ILE:HD13	1.90	0.52
1:C:64:GLY:HA3	1:C:208:TYR:HB3	1.92	0.52
1:B:228:ILE:HD13	1:B:228:ILE:H	1.74	0.52
1:A:241:PRO:HD3	1:A:247:ALA:CB	2.40	0.52
1:A:209:ILE:N	1:A:209:ILE:HD12	2.25	0.52
1:A:386:CYS:SG	1:A:408:ALA:HB3	2.50	0.52
1:D:357:ALA:HA	1:D:367:GLY:HA3	1.90	0.52
1:C:305:THR:HG22	1:C:306:TYR:H	1.74	0.52
1:D:251:ILE:HD12	1:D:251:ILE:N	2.24	0.52
1:D:241:PRO:CG	1:D:247:ALA:H	2.23	0.52
1:D:257:HIS:CE1	1:D:437:ASN:HB2	2.45	0.52
4:B:540:NAG:O3	3:B:541:MAN:O5	2.28	0.51
1:C:135:TRP:HB3	1:C:139:GLU:HG2	1.90	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:400:THR:CG2	1:D:401:GLU:N	2.73	0.51
1:B:244:THR:O	1:B:244:THR:HG22	2.10	0.51
1:C:56:VAL:HG11	1:C:202:MET:CE	2.40	0.51
1:C:320:LEU:HD22	1:C:374:ILE:HD13	1.92	0.51
1:C:233:PHE:CG	1:C:234:THR:N	2.77	0.51
1:D:281:ILE:HD11	1:D:396:VAL:HB	1.93	0.51
1:A:135:TRP:CG	1:A:139:GLU:HG3	2.44	0.51
1:A:67:ILE:HD11	1:A:163:LEU:HD12	1.92	0.51
1:A:400:THR:CG2	1:A:401:GLU:N	2.73	0.51
1:D:320:LEU:HD22	1:D:374:ILE:HD13	1.91	0.51
1:C:46:ILE:HD13	1:C:202:MET:HE2	1.92	0.51
1:C:93:LEU:HD21	1:C:177:PHE:CD2	2.36	0.51
1:D:400:THR:HG22	1:D:401:GLU:N	2.26	0.51
1:B:74:PHE:CE2	1:B:92:LEU:HD13	2.44	0.51
1:A:74:PHE:CE2	1:A:92:LEU:HD13	2.45	0.51
1:B:257:HIS:CE1	1:B:437:ASN:HB2	2.46	0.51
1:C:94:GLN:HA	1:C:110:ASN:ND2	2.26	0.51
1:D:425:ARG:HG2	1:D:432:GLY:O	2.11	0.51
1:A:56:VAL:HG11	1:A:202:MET:CE	2.41	0.51
1:A:56:VAL:HG11	1:A:202:MET:HE3	1.92	0.51
1:A:241:PRO:CG	1:A:247:ALA:H	2.23	0.51
1:C:436:ALA:O	1:C:437:ASN:CB	2.59	0.51
1:B:400:THR:CG2	1:B:401:GLU:N	2.73	0.51
1:D:395:ALA:HB1	4:D:740:NAG:H82	1.91	0.51
1:C:357:ALA:HA	1:C:367:GLY:HA3	1.92	0.51
1:C:244:THR:HG22	1:C:244:THR:O	2.11	0.51
1:A:233:PHE:CG	1:A:234:THR:N	2.78	0.51
1:A:406:ASN:CG	2:A:442:NDG:H1L	2.11	0.51
1:A:388:ILE:HG12	4:A:440:NAG:O1	2.11	0.51
1:D:238:THR:HG22	1:D:239:ALA:N	2.25	0.51
1:D:101:GLY:HA3	1:D:171:HIS:CD2	2.46	0.51
1:A:216:ARG:NH1	1:A:216:ARG:HG2	2.23	0.50
1:B:56:VAL:HG11	1:B:202:MET:CE	2.41	0.50
1:B:94:GLN:HA	1:B:110:ASN:ND2	2.26	0.50
1:C:101:GLY:HA3	1:C:171:HIS:CD2	2.46	0.50
1:B:280:ASN:ND2	2:B:538:NDG:C5	2.73	0.50
1:D:276:THR:HG23	1:D:310:LEU:HB3	1.92	0.50
1:B:357:ALA:HA	1:B:367:GLY:HA3	1.92	0.50
1:B:278:LEU:HD21	1:B:298:PRO:HB3	1.92	0.50
1:C:258:PRO:HB3	1:C:368:THR:CG2	2.41	0.50
1:B:218:ARG:HB3	1:B:218:ARG:NH1	2.26	0.50
1:C:406:ASN:ND2	2:C:642:NDG:C1	2.74	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:400:THR:HG22	1:B:401:GLU:N	2.27	0.50
4:C:640:NAG:O3	3:C:641:MAN:O5	2.28	0.50
1:D:135:TRP:HB3	1:D:139:GLU:HG2	1.91	0.50
1:D:241:PRO:HG3	1:D:247:ALA:H	1.77	0.50
1:C:241:PRO:CG	1:C:247:ALA:H	2.24	0.50
1:A:238:THR:HG22	1:A:239:ALA:N	2.26	0.50
1:B:370:ASN:C	1:B:370:ASN:HD22	2.14	0.50
1:A:400:THR:HG22	1:A:401:GLU:N	2.26	0.50
1:D:233:PHE:CG	1:D:234:THR:N	2.79	0.50
1:B:395:ALA:O	1:B:399:ASN:ND2	2.43	0.50
1:A:436:ALA:O	1:A:437:ASN:CB	2.59	0.50
1:B:436:ALA:O	1:B:437:ASN:CB	2.60	0.50
1:B:281:ILE:HD11	1:B:396:VAL:HB	1.93	0.50
1:B:233:PHE:CG	1:B:234:THR:N	2.79	0.50
1:A:84:THR:O	1:A:84:THR:HG22	2.12	0.50
1:A:166:ILE:HD11	1:A:219:PHE:HB3	1.93	0.50
1:B:258:PRO:HB3	1:B:368:THR:CG2	2.42	0.50
1:D:392:SER:O	1:D:396:VAL:HG23	2.12	0.50
1:D:166:ILE:HD11	1:D:219:PHE:HB3	1.94	0.50
1:B:91:GLU:HA	1:B:110:ASN:OD1	2.12	0.50
1:D:244:THR:HG22	1:D:244:THR:O	2.11	0.50
1:A:47:ASN:O	1:A:56:VAL:HG23	2.11	0.50
1:A:357:ALA:HA	1:A:367:GLY:HA3	1.93	0.50
1:D:50:VAL:HG22	1:D:202:MET:HE2	1.94	0.49
1:C:238:THR:HG22	1:C:239:ALA:N	2.27	0.49
1:C:281:ILE:HD11	1:C:396:VAL:HB	1.94	0.49
1:A:111:ASP:HB3	1:A:417:TYR:OH	2.12	0.49
1:A:342:SER:HB2	1:A:360:PRO:CD	2.42	0.49
1:C:280:ASN:OD1	2:C:638:NDG:C1	2.60	0.49
2:A:438:NDG:C4	3:A:439:MAN:C2	2.86	0.49
1:C:241:PRO:HD3	1:C:247:ALA:CB	2.41	0.49
1:D:342:SER:HB2	1:D:360:PRO:CD	2.42	0.49
1:C:145:LYS:HD3	1:C:147:PHE:CE2	2.47	0.49
1:C:241:PRO:HG3	1:C:247:ALA:H	1.77	0.49
1:C:436:ALA:O	1:C:437:ASN:CG	2.51	0.49
1:D:67:ILE:HD11	1:D:163:LEU:HD12	1.95	0.49
1:A:353:LEU:HD22	1:A:354:TYR:N	2.28	0.49
1:A:406:ASN:CG	2:A:442:NDG:C1	2.80	0.49
1:B:101:GLY:HA3	1:B:171:HIS:CD2	2.48	0.49
1:C:74:PHE:CE2	1:C:92:LEU:HD13	2.47	0.49
1:B:111:ASP:HB3	1:B:417:TYR:OH	2.11	0.49
1:D:135:TRP:HB3	1:D:139:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:216:ARG:CG	1:D:216:ARG:NH1	2.72	0.49
1:C:242:SER:O	1:C:243:ALA:CB	2.59	0.49
1:A:265:ASN:HD22	1:A:265:ASN:C	2.16	0.49
2:B:538:NDG:C4	3:B:539:MAN:C2	2.88	0.49
1:A:256:ASN:ND2	1:A:437:ASN:HB3	2.27	0.49
1:B:256:ASN:ND2	1:B:437:ASN:HB3	2.28	0.49
1:C:294:THR:HG22	1:C:296:THR:H	1.76	0.49
1:D:111:ASP:HB3	1:D:417:TYR:OH	2.12	0.49
1:D:388:ILE:HG12	4:D:740:NAG:O1	2.13	0.49
1:B:56:VAL:HG13	1:B:177:PHE:HB2	1.94	0.49
1:B:342:SER:HB2	1:B:360:PRO:CD	2.43	0.49
1:C:84:THR:HG22	1:C:84:THR:O	2.11	0.49
1:C:395:ALA:HB1	4:C:640:NAG:H82	1.93	0.49
1:B:395:ALA:HB1	4:B:540:NAG:H82	1.95	0.49
1:D:414:LEU:HD22	1:D:416:ILE:HG13	1.94	0.49
1:B:241:PRO:CG	1:B:247:ALA:H	2.26	0.49
1:C:370:ASN:ND2	1:C:372:SER:HB2	2.28	0.49
1:D:353:LEU:HD22	1:D:354:TYR:N	2.27	0.49
1:A:182:GLN:HA	1:A:187:ASN:HD22	1.77	0.49
1:D:84:THR:O	1:D:84:THR:HG22	2.13	0.49
1:A:290:THR:HG23	1:A:292:ALA:N	2.13	0.49
4:C:640:NAG:H3	3:C:641:MAN:H1	1.95	0.49
1:D:218:ARG:NH1	1:D:218:ARG:HB3	2.27	0.49
1:C:406:ASN:CG	2:C:642:NDG:C1	2.81	0.48
1:D:47:ASN:O	1:D:56:VAL:HG23	2.13	0.48
1:C:146:ARG:CG	1:C:146:ARG:NH1	2.75	0.48
1:A:243:ALA:C	1:A:245:THR:N	2.65	0.48
1:A:228:ILE:H	1:A:228:ILE:HD13	1.76	0.48
1:C:256:ASN:ND2	1:C:437:ASN:HB3	2.28	0.48
1:B:401:GLU:O	1:B:401:GLU:HG2	2.12	0.48
1:A:94:GLN:HA	1:A:110:ASN:ND2	2.28	0.48
1:C:342:SER:HB2	1:C:360:PRO:CD	2.43	0.48
1:D:134:ASP:HA	1:D:147:PHE:HE2	1.78	0.48
1:B:46:ILE:HD13	1:B:202:MET:HE2	1.93	0.48
1:D:243:ALA:C	1:D:245:THR:N	2.67	0.48
1:B:241:PRO:HD3	1:B:247:ALA:CB	2.42	0.48
1:D:94:GLN:HA	1:D:110:ASN:ND2	2.28	0.48
1:C:229:GLU:HA	1:C:420:ASN:O	2.14	0.48
1:D:260:LYS:HG2	1:D:421:TYR:CE2	2.48	0.48
1:B:406:ASN:CG	2:B:542:NDG:C1	2.81	0.48
1:D:78:LYS:HD3	1:D:139:GLU:HB2	1.95	0.48
1:C:228:ILE:HD13	1:C:228:ILE:H	1.77	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:252:ARG:CZ	1:D:376:ASN:HD22	2.27	0.48
1:C:135:TRP:HB3	1:C:139:GLU:HG3	1.96	0.48
1:D:399:ASN:ND2	4:D:740:NAG:O5	2.46	0.48
1:A:166:ILE:HD11	1:A:219:PHE:CB	2.44	0.48
1:A:241:PRO:CB	1:A:245:THR:O	2.60	0.48
1:B:229:GLU:HA	1:B:420:ASN:O	2.14	0.48
1:A:281:ILE:HD11	1:A:396:VAL:HB	1.96	0.48
1:C:399:ASN:ND2	4:C:640:NAG:O5	2.47	0.48
1:A:257:HIS:CE1	1:A:437:ASN:HB2	2.49	0.48
1:A:172:GLU:OE1	1:A:174:LYS:CD	2.61	0.48
1:A:401:GLU:HG2	1:A:401:GLU:O	2.13	0.48
1:C:392:SER:O	1:C:396:VAL:HG23	2.13	0.48
1:D:229:GLU:HA	1:D:420:ASN:O	2.14	0.48
1:C:370:ASN:C	1:C:370:ASN:HD22	2.18	0.48
1:B:47:ASN:O	1:B:56:VAL:HG23	2.13	0.47
1:D:242:SER:O	1:D:243:ALA:CB	2.62	0.47
1:A:241:PRO:HG3	1:A:247:ALA:H	1.78	0.47
1:B:243:ALA:C	1:B:245:THR:N	2.67	0.47
1:D:436:ALA:O	1:D:437:ASN:CB	2.62	0.47
1:D:278:LEU:HD21	1:D:298:PRO:HB3	1.95	0.47
2:D:738:NDG:C4	3:D:739:MAN:C2	2.88	0.47
1:D:406:ASN:ND2	2:D:742:NDG:C1	2.74	0.47
4:D:740:NAG:O3	3:D:741:MAN:O5	2.31	0.47
1:B:46:ILE:CD1	1:B:202:MET:HG2	2.44	0.47
1:B:425:ARG:HG2	1:B:432:GLY:O	2.14	0.47
1:D:228:ILE:H	1:D:228:ILE:HD13	1.78	0.47
4:A:440:NAG:H3	3:A:441:MAN:H1	1.95	0.47
1:B:278:LEU:HB2	1:B:407:THR:HG21	1.96	0.47
1:D:252:ARG:CZ	1:D:376:ASN:ND2	2.78	0.47
1:D:187:ASN:ND2	1:D:188:TYR:CE1	2.83	0.47
1:A:104:ARG:CD	1:D:102:GLY:HA3	2.35	0.47
1:C:243:ALA:HA	1:C:385:THR:CG2	2.45	0.47
1:A:228:ILE:HD13	1:A:422:ASN:O	2.14	0.47
1:B:187:ASN:ND2	1:B:188:TYR:CE1	2.83	0.47
1:D:290:THR:HG23	1:D:292:ALA:N	2.14	0.47
4:D:740:NAG:H3	3:D:741:MAN:H1	1.97	0.47
1:C:265:ASN:HD22	1:C:265:ASN:C	2.17	0.47
1:B:228:ILE:HD13	1:B:422:ASN:O	2.14	0.47
1:A:406:ASN:ND2	2:A:442:NDG:C1	2.77	0.47
4:B:540:NAG:H3	3:B:541:MAN:H1	1.95	0.47
1:C:166:ILE:HD11	1:C:219:PHE:HB3	1.94	0.47
1:A:258:PRO:HB3	1:A:368:THR:CG2	2.42	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:GLY:HA3	1:A:171:HIS:CD2	2.48	0.47
1:A:293:ALA:HB3	2:A:438:NDG:O6	2.15	0.47
1:A:134:ASP:HA	1:A:147:PHE:HE2	1.78	0.47
1:C:399:ASN:ND2	4:C:640:NAG:C1	2.73	0.47
1:B:166:ILE:HD11	1:B:219:PHE:HB3	1.95	0.47
1:D:91:GLU:HA	1:D:110:ASN:OD1	2.15	0.47
1:A:218:ARG:NH1	1:A:218:ARG:HB3	2.28	0.47
1:A:252:ARG:CZ	1:A:376:ASN:HD22	2.28	0.47
2:A:438:NDG:O4	3:A:439:MAN:O2	2.31	0.47
1:B:216:ARG:HG2	1:B:216:ARG:NH1	2.21	0.47
1:A:146:ARG:CG	1:A:146:ARG:NH1	2.78	0.47
1:D:337:VAL:O	1:D:341:GLN:HG3	2.15	0.47
1:D:406:ASN:CG	2:D:742:NDG:C1	2.83	0.47
1:A:436:ALA:O	1:A:437:ASN:CG	2.54	0.47
1:C:172:GLU:OE1	1:C:174:LYS:CD	2.63	0.47
2:D:738:NDG:O6	3:D:739:MAN:H2	2.14	0.47
1:B:145:LYS:HD3	1:B:147:PHE:CE2	2.49	0.47
1:B:399:ASN:ND2	4:B:540:NAG:O5	2.48	0.47
1:A:78:LYS:NZ	6:A:464:HOH:O	2.42	0.47
1:D:243:ALA:HA	1:D:385:THR:CG2	2.45	0.47
2:D:738:NDG:H1	2:D:738:NDG:O7	2.14	0.46
1:A:135:TRP:HB3	1:A:139:GLU:HG3	1.98	0.46
1:A:414:LEU:HD22	1:A:416:ILE:HG13	1.97	0.46
1:A:252:ARG:CZ	1:A:376:ASN:ND2	2.78	0.46
2:C:638:NDG:O7	2:C:638:NDG:H1	2.15	0.46
1:B:50:VAL:HG22	1:B:202:MET:HE2	1.96	0.46
1:B:238:THR:HG22	1:B:239:ALA:N	2.29	0.46
1:C:233:PHE:CD1	1:C:234:THR:N	2.84	0.46
1:A:145:LYS:HD3	1:A:147:PHE:CE2	2.51	0.46
1:B:290:THR:HG23	1:B:292:ALA:N	2.16	0.46
1:C:238:THR:OG1	1:C:266:PHE:HD2	1.99	0.46
1:C:401:GLU:O	1:C:401:GLU:HG2	2.15	0.46
1:B:406:ASN:ND2	2:B:542:NDG:C1	2.76	0.46
1:C:243:ALA:C	1:C:245:THR:N	2.66	0.46
1:B:436:ALA:O	1:B:437:ASN:CG	2.54	0.46
2:B:538:NDG:O6	3:B:539:MAN:H2	2.15	0.46
1:A:84:THR:HB	6:A:464:HOH:O	2.16	0.46
1:D:265:ASN:HD22	1:D:265:ASN:C	2.18	0.46
1:D:258:PRO:HB3	1:D:368:THR:CG2	2.41	0.46
1:D:280:ASN:ND2	2:D:738:NDG:O	2.46	0.46
1:B:395:ALA:HB2	4:B:540:NAG:H82	1.97	0.46
1:C:166:ILE:HD11	1:C:219:PHE:CB	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:216:ARG:NH1	1:C:216:ARG:CG	2.74	0.46
1:B:241:PRO:HG3	1:B:247:ALA:H	1.80	0.46
1:D:199:GLN:N	1:D:199:GLN:CD	2.69	0.46
1:D:238:THR:OG1	1:D:266:PHE:HD2	1.99	0.46
1:C:425:ARG:HG2	1:C:432:GLY:O	2.16	0.46
1:C:280:ASN:ND2	2:C:638:NDG:H5	2.30	0.46
1:D:381:LEU:HD11	1:D:414:LEU:HD11	1.98	0.46
1:C:257:HIS:CE1	1:C:437:ASN:HB2	2.50	0.46
1:A:370:ASN:HD22	1:A:370:ASN:C	2.18	0.46
1:B:108:HIS:HB3	1:B:113:PHE:HE1	1.81	0.46
1:C:252:ARG:CZ	1:C:376:ASN:ND2	2.79	0.46
1:A:381:LEU:HD11	1:A:414:LEU:HD11	1.98	0.46
1:D:172:GLU:OE1	1:D:174:LYS:CD	2.63	0.46
1:C:278:LEU:HD21	1:C:298:PRO:HB3	1.97	0.46
1:A:280:ASN:OD1	2:A:438:NDG:C1	2.64	0.46
1:A:216:ARG:CG	1:A:216:ARG:NH1	2.75	0.46
1:C:388:ILE:HG12	4:C:640:NAG:O1	2.16	0.45
1:C:241:PRO:HB3	1:C:245:THR:HG23	1.98	0.45
1:B:242:SER:O	1:B:243:ALA:CB	2.64	0.45
1:A:91:GLU:HA	1:A:110:ASN:OD1	2.16	0.45
1:B:182:GLN:HA	1:B:187:ASN:HD22	1.81	0.45
1:A:229:GLU:HA	1:A:420:ASN:O	2.16	0.45
1:B:135:TRP:HB3	1:B:139:GLU:HG3	1.97	0.45
1:C:414:LEU:HD22	1:C:416:ILE:HG13	1.97	0.45
1:A:108:HIS:HD2	6:A:456:HOH:O	1.99	0.45
1:D:166:ILE:HD11	1:D:219:PHE:CB	2.47	0.45
1:B:166:ILE:HD11	1:B:219:PHE:CB	2.46	0.45
1:A:306:TYR:CD2	1:A:348:PRO:HA	2.52	0.45
1:C:67:ILE:HD11	1:C:163:LEU:HD12	1.97	0.45
1:C:252:ARG:CZ	1:C:376:ASN:HD22	2.30	0.45
1:C:65:ASP:OD1	1:C:216:ARG:NH1	2.50	0.45
1:A:46:ILE:CD1	1:A:202:MET:HG2	2.47	0.45
4:C:640:NAG:C3	3:C:641:MAN:C1	2.94	0.45
1:B:388:ILE:HG12	4:B:540:NAG:O1	2.17	0.45
1:C:78:LYS:HD3	1:C:139:GLU:HB2	1.97	0.45
1:A:241:PRO:HB3	1:A:245:THR:HG23	1.99	0.45
1:B:353:LEU:HD22	1:B:354:TYR:H	1.80	0.45
1:A:187:ASN:ND2	1:A:188:TYR:CE1	2.85	0.45
1:C:353:LEU:HD22	1:C:354:TYR:N	2.31	0.45
1:D:267:ASN:O	1:D:269:PRO:HD3	2.17	0.45
1:C:338:GLN:CB	1:C:339:PRO:HD3	2.47	0.45
1:D:46:ILE:CD1	1:D:202:MET:HG2	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:46:ILE:CD1	1:C:202:MET:HG2	2.47	0.45
1:B:75:VAL:CG2	1:B:146:ARG:NH1	2.80	0.45
1:C:238:THR:CG2	1:C:239:ALA:N	2.80	0.45
1:D:370:ASN:ND2	1:D:372:SER:HB2	2.32	0.45
1:C:199:GLN:N	1:C:199:GLN:CD	2.70	0.45
1:A:337:VAL:O	1:A:341:GLN:HG3	2.17	0.45
2:A:438:NDG:H1	2:A:438:NDG:O7	2.17	0.45
1:C:145:LYS:HB3	1:C:147:PHE:CZ	2.52	0.45
1:A:406:ASN:C	2:A:442:NDG:H8C3	2.35	0.45
1:D:75:VAL:CG2	1:D:146:ARG:NH1	2.80	0.45
1:A:55:LYS:HE2	1:D:47:ASN:ND2	2.32	0.45
1:A:238:THR:CG2	1:A:239:ALA:N	2.80	0.45
1:D:401:GLU:O	1:D:401:GLU:HG2	2.16	0.45
1:A:199:GLN:CD	1:A:199:GLN:N	2.70	0.45
1:A:108:HIS:HB3	1:A:113:PHE:HE1	1.80	0.45
1:C:395:ALA:HB2	4:C:640:NAG:H82	1.98	0.45
1:B:135:TRP:HD1	1:B:139:GLU:HG3	1.78	0.45
1:A:399:ASN:ND2	4:A:440:NAG:O5	2.50	0.45
1:D:278:LEU:HB2	1:D:407:THR:HG21	1.99	0.45
1:C:278:LEU:HB2	1:C:407:THR:HG21	1.97	0.45
1:D:395:ALA:HB2	4:D:740:NAG:H82	1.98	0.44
1:D:46:ILE:HD13	1:D:202:MET:HE2	1.99	0.44
1:D:241:PRO:HD3	1:D:247:ALA:CB	2.46	0.44
1:A:238:THR:OG1	1:A:266:PHE:HD2	2.00	0.44
1:B:252:ARG:CZ	1:B:376:ASN:ND2	2.80	0.44
1:B:134:ASP:HA	1:B:147:PHE:HE2	1.80	0.44
1:C:47:ASN:O	1:C:56:VAL:HG23	2.18	0.44
1:B:46:ILE:HD11	1:B:202:MET:HG2	1.98	0.44
1:C:50:VAL:HG22	1:C:202:MET:HE2	1.99	0.44
1:C:46:ILE:HD11	1:C:202:MET:HG2	1.99	0.44
1:C:56:VAL:HG13	1:C:177:PHE:HB2	2.00	0.44
1:B:414:LEU:HD22	1:B:416:ILE:HG13	1.98	0.44
1:B:252:ARG:CZ	1:B:376:ASN:HD22	2.30	0.44
1:A:260:LYS:HG2	1:A:421:TYR:CE2	2.52	0.44
1:A:280:ASN:ND2	2:A:438:NDG:O	2.50	0.44
1:C:88:PRO:CD	1:C:134:ASP:CB	2.90	0.44
1:A:65:ASP:OD1	1:A:216:ARG:NH1	2.50	0.44
1:B:265:ASN:C	1:B:265:ASN:HD22	2.20	0.44
1:C:108:HIS:HB3	1:C:113:PHE:HE1	1.83	0.44
1:A:395:ALA:HB2	4:A:440:NAG:H82	1.99	0.44
1:A:46:ILE:HD11	1:A:204:VAL:HG23	2.00	0.44
1:B:381:LEU:HD11	1:B:414:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:ASN:C	1:A:265:ASN:ND2	2.70	0.44
1:D:223:PRO:HB3	1:D:427:MET:CE	2.48	0.44
1:D:56:VAL:HG13	1:D:177:PHE:HB2	1.99	0.44
1:B:392:SER:O	1:B:396:VAL:HG23	2.17	0.44
4:B:540:NAG:C3	3:B:541:MAN:C1	2.96	0.44
1:A:78:LYS:HD3	1:A:139:GLU:HB2	2.00	0.44
1:C:66:LEU:HD23	1:C:164:PRO:HA	1.99	0.44
1:D:238:THR:CG2	1:D:239:ALA:N	2.80	0.44
1:B:238:THR:HG23	1:B:383:TYR:CZ	2.53	0.44
1:C:120:PHE:HD2	1:C:361:ALA:HB2	1.83	0.44
1:C:295:VAL:O	1:C:295:VAL:CG1	2.65	0.44
1:D:223:PRO:HB3	1:D:427:MET:HE3	1.99	0.44
1:C:260:LYS:HG2	1:C:421:TYR:CE2	2.53	0.44
1:B:85:THR:HG23	1:B:88:PRO:HD3	1.99	0.44
1:A:243:ALA:HA	1:A:385:THR:CG2	2.48	0.44
1:C:241:PRO:CB	1:C:245:THR:O	2.62	0.44
1:D:295:VAL:O	1:D:295:VAL:CG1	2.66	0.44
1:A:85:THR:HG23	1:A:88:PRO:HD3	2.01	0.43
1:B:399:ASN:ND2	4:B:540:NAG:C1	2.74	0.43
1:B:56:VAL:HG11	1:B:202:MET:HE3	1.99	0.43
1:B:243:ALA:HA	1:B:385:THR:CG2	2.48	0.43
1:C:187:ASN:ND2	1:C:188:TYR:CE1	2.86	0.43
1:A:56:VAL:HG13	1:A:177:PHE:HB2	2.00	0.43
1:B:61:SER:OG	1:B:63:ASN:ND2	2.50	0.43
1:A:370:ASN:ND2	1:A:372:SER:HB2	2.30	0.43
1:B:66:LEU:HD23	1:B:164:PRO:HA	2.00	0.43
1:D:108:HIS:HB3	1:D:113:PHE:HE1	1.83	0.43
1:C:75:VAL:CG2	1:C:146:ARG:NH1	2.80	0.43
1:D:56:VAL:HG11	1:D:202:MET:HE3	2.01	0.43
1:D:44:GLN:HE21	1:D:61:SER:H	1.65	0.43
1:B:370:ASN:ND2	1:B:372:SER:HB2	2.31	0.43
1:A:295:VAL:O	1:A:295:VAL:CG1	2.65	0.43
1:A:353:LEU:HD22	1:A:354:TYR:H	1.83	0.43
1:D:182:GLN:HA	1:D:187:ASN:HD22	1.84	0.43
1:C:32:ARG:NH1	1:C:32:ARG:HG3	2.34	0.43
1:A:223:PRO:HB3	1:A:427:MET:CE	2.47	0.43
1:A:425:ARG:HG2	1:A:432:GLY:O	2.18	0.43
1:B:78:LYS:HD3	1:B:139:GLU:HB2	2.00	0.43
4:A:440:NAG:C3	3:A:441:MAN:C1	2.96	0.43
1:A:55:LYS:HE2	1:D:47:ASN:HD21	1.82	0.43
1:B:238:THR:OG1	1:B:266:PHE:HD2	2.00	0.43
1:D:436:ALA:O	1:D:437:ASN:CG	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:740:NAG:H82	4:D:740:NAG:H1	2.00	0.43
1:D:238:THR:HG23	1:D:383:TYR:CZ	2.53	0.43
1:C:381:LEU:HD11	1:C:414:LEU:HD11	2.00	0.43
1:D:370:ASN:C	1:D:370:ASN:HD22	2.21	0.43
1:A:278:LEU:HB2	1:A:407:THR:HG21	1.99	0.43
1:A:269:PRO:HG3	1:A:413:ALA:HB2	2.01	0.43
1:B:84:THR:O	1:B:84:THR:HG22	2.18	0.43
1:C:280:ASN:ND2	2:C:638:NDG:O	2.51	0.43
1:B:65:ASP:OD1	1:B:216:ARG:NH1	2.52	0.43
1:B:236:SER:HB2	1:B:414:LEU:HB3	2.01	0.43
1:B:174:LYS:HZ3	1:B:174:LYS:HB3	1.83	0.43
1:C:32:ARG:HG3	1:C:32:ARG:HH11	1.83	0.43
1:D:46:ILE:HD11	1:D:204:VAL:HG23	2.00	0.43
1:A:75:VAL:CG2	1:A:146:ARG:NH1	2.82	0.43
1:D:145:LYS:HB3	1:D:147:PHE:CZ	2.53	0.43
1:B:266:PHE:CE2	1:B:414:LEU:HG	2.53	0.43
1:A:276:THR:HB	6:A:468:HOH:O	2.18	0.43
1:B:294:THR:HG22	1:B:296:THR:HB	2.01	0.43
1:A:233:PHE:CD1	1:A:234:THR:N	2.85	0.43
1:D:187:ASN:ND2	1:D:188:TYR:HE1	2.17	0.43
1:C:269:PRO:HG3	1:C:413:ALA:HB2	1.99	0.43
4:D:740:NAG:C3	3:D:741:MAN:C1	2.96	0.43
1:C:236:SER:HB2	1:C:414:LEU:HB3	2.01	0.43
1:A:61:SER:OG	1:A:63:ASN:ND2	2.50	0.43
1:A:342:SER:HB2	1:A:360:PRO:HD2	2.01	0.43
1:B:223:PRO:HB3	1:B:427:MET:CE	2.49	0.43
1:C:238:THR:HG23	1:C:383:TYR:CZ	2.54	0.43
1:B:199:GLN:CD	1:B:199:GLN:N	2.70	0.43
1:A:294:THR:HG22	1:A:296:THR:HB	2.01	0.43
1:D:342:SER:HB2	1:D:360:PRO:HD2	2.00	0.43
1:C:267:ASN:O	1:C:269:PRO:HD3	2.19	0.43
1:D:32:ARG:NH1	1:D:32:ARG:HG3	2.34	0.43
1:B:87:TYR:CD2	1:B:133:THR:HG21	2.47	0.42
1:D:146:ARG:CG	1:D:146:ARG:NH1	2.77	0.42
1:A:238:THR:HG23	1:A:383:TYR:CZ	2.53	0.42
1:D:231:LEU:HD22	1:D:232:GLN:H	1.84	0.42
1:B:295:VAL:CG1	1:B:295:VAL:O	2.67	0.42
1:B:187:ASN:ND2	1:B:188:TYR:HE1	2.17	0.42
1:D:32:ARG:HH11	1:D:32:ARG:HG3	1.84	0.42
1:B:306:TYR:CD2	1:B:348:PRO:HA	2.55	0.42
1:D:153:PHE:H	1:D:156:ASN:ND2	2.02	0.42
1:C:46:ILE:HD13	1:C:202:MET:CE	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:231:LEU:HD22	1:C:232:GLN:H	1.84	0.42
1:B:233:PHE:CD1	1:B:234:THR:N	2.85	0.42
1:A:32:ARG:HG3	1:A:32:ARG:HH11	1.84	0.42
1:D:88:PRO:CD	1:D:134:ASP:CB	2.87	0.42
1:D:87:TYR:N	1:D:88:PRO:CD	2.82	0.42
1:B:44:GLN:HE21	1:B:61:SER:H	1.65	0.42
1:A:338:GLN:CB	1:A:339:PRO:HD3	2.46	0.42
1:C:309:GLN:NE2	1:C:403:VAL:O	2.52	0.42
1:D:46:ILE:HD11	1:D:202:MET:HG2	2.00	0.42
1:B:269:PRO:HG3	1:B:413:ALA:HB2	2.01	0.42
1:D:133:THR:CG2	1:D:133:THR:O	2.67	0.42
1:C:228:ILE:HD13	1:C:422:ASN:O	2.19	0.42
1:A:392:SER:O	1:A:396:VAL:HG23	2.19	0.42
1:C:337:VAL:O	1:C:341:GLN:HG3	2.20	0.42
1:A:242:SER:O	1:A:243:ALA:CB	2.60	0.42
1:C:266:PHE:CE2	1:C:414:LEU:HG	2.55	0.42
1:A:390:ALA:HB2	1:A:405:ALA:HB1	2.01	0.42
1:D:65:ASP:OD1	1:D:216:ARG:NH1	2.52	0.42
1:B:238:THR:CG2	1:B:239:ALA:N	2.83	0.42
1:D:266:PHE:CE2	1:D:414:LEU:HG	2.54	0.42
1:A:384:LYS:HB3	1:A:402:THR:O	2.20	0.42
1:D:357:ALA:HB2	1:D:367:GLY:O	2.20	0.42
1:B:145:LYS:HB3	1:B:147:PHE:CZ	2.54	0.42
1:D:309:GLN:NE2	1:D:403:VAL:O	2.53	0.42
1:D:388:ILE:HB	1:D:405:ALA:HA	2.02	0.42
1:B:32:ARG:HG3	1:B:32:ARG:NH1	2.35	0.42
1:D:241:PRO:HB3	1:D:245:THR:HG23	2.01	0.42
1:B:241:PRO:HB3	1:B:245:THR:HG23	2.01	0.42
1:A:145:LYS:HB3	1:A:147:PHE:CZ	2.55	0.41
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.84	0.41
1:D:280:ASN:OD1	2:D:738:NDG:C1	2.68	0.41
1:B:388:ILE:HB	1:B:405:ALA:HA	2.03	0.41
1:D:399:ASN:ND2	4:D:740:NAG:O1	2.47	0.41
1:D:265:ASN:ND2	1:D:265:ASN:C	2.73	0.41
1:D:294:THR:HG22	1:D:296:THR:HB	2.02	0.41
1:B:342:SER:HB2	1:B:360:PRO:HD2	2.02	0.41
1:A:32:ARG:NH1	1:A:32:ARG:HG3	2.35	0.41
1:C:87:TYR:N	1:C:88:PRO:CD	2.82	0.41
1:A:399:ASN:ND2	4:A:440:NAG:C1	2.73	0.41
1:A:312:VAL:HG13	1:A:411:LEU:HD12	2.02	0.41
1:C:182:GLN:HA	1:C:187:ASN:HD22	1.85	0.41
1:D:395:ALA:HB1	4:D:740:NAG:H1	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:ASN:ND2	1:D:55:LYS:HE2	2.30	0.41
1:B:172:GLU:OE1	1:B:174:LYS:CD	2.66	0.41
1:C:265:ASN:C	1:C:265:ASN:ND2	2.72	0.41
1:B:281:ILE:HD12	1:B:396:VAL:HG11	2.02	0.41
1:A:187:ASN:ND2	1:A:188:TYR:HE1	2.19	0.41
1:B:337:VAL:O	1:B:341:GLN:HG3	2.20	0.41
1:C:223:PRO:HB3	1:C:427:MET:CE	2.51	0.41
1:B:120:PHE:HD2	1:B:361:ALA:HB2	1.86	0.41
1:D:87:TYR:CD2	1:D:133:THR:HG21	2.52	0.41
1:D:306:TYR:CD2	1:D:348:PRO:HA	2.56	0.41
1:B:50:VAL:HG22	1:B:202:MET:HE1	2.03	0.41
1:D:241:PRO:CB	1:D:245:THR:O	2.61	0.41
1:D:66:LEU:HD23	1:D:164:PRO:HA	2.02	0.41
1:B:251:ILE:HD12	1:B:251:ILE:H	1.85	0.41
1:B:267:ASN:O	1:B:269:PRO:HD3	2.21	0.41
1:B:46:ILE:HD11	1:B:204:VAL:HG23	2.02	0.41
1:D:242:SER:HA	5:D:744:HG:HG	1.80	0.41
1:A:236:SER:HB2	1:A:414:LEU:HB3	2.03	0.41
1:D:353:LEU:HD22	1:D:354:TYR:H	1.85	0.41
1:D:170:TYR:CD1	1:D:429:GLY:HA3	2.56	0.41
1:D:280:ASN:ND2	2:D:738:NDG:H5	2.33	0.41
1:A:389:ASP:N	4:A:440:NAG:O7	2.54	0.41
1:A:266:PHE:CE2	1:A:414:LEU:HG	2.55	0.41
1:B:44:GLN:HB3	1:B:58:THR:HG21	2.02	0.41
1:C:342:SER:HB2	1:C:360:PRO:HD2	2.02	0.41
1:C:353:LEU:HD22	1:C:354:TYR:H	1.86	0.41
1:D:269:PRO:HG3	1:D:413:ALA:HB2	2.03	0.41
1:D:406:ASN:OD1	2:D:742:NDG:O1L	2.26	0.41
1:A:50:VAL:HG22	1:A:202:MET:HE1	2.01	0.41
1:D:233:PHE:CD1	1:D:234:THR:N	2.86	0.41
1:A:120:PHE:HD2	1:A:361:ALA:HB2	1.86	0.41
1:B:28:LYS:HD2	1:B:28:LYS:HA	1.95	0.41
1:A:133:THR:O	1:A:133:THR:CG2	2.69	0.41
1:B:88:PRO:CD	1:B:134:ASP:CB	2.90	0.41
1:C:216:ARG:NH1	1:C:216:ARG:HG2	2.22	0.41
1:C:46:ILE:HD11	1:C:204:VAL:HG23	2.02	0.41
1:B:312:VAL:HG13	1:B:411:LEU:HD12	2.03	0.41
1:B:338:GLN:CB	1:B:339:PRO:HD3	2.49	0.41
1:A:199:GLN:O	1:A:199:GLN:NE2	2.54	0.41
1:C:294:THR:HG22	1:C:296:THR:HB	2.03	0.41
1:D:120:PHE:HD2	1:D:361:ALA:HB2	1.85	0.41
1:C:406:ASN:C	2:C:642:NDG:H8C3	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:216:ARG:CG	1:B:216:ARG:NH1	2.74	0.40
1:A:267:ASN:O	1:A:269:PRO:HD3	2.21	0.40
1:A:60:ILE:HD12	1:A:206:VAL:HG21	2.02	0.40
1:B:260:LYS:HG2	1:B:421:TYR:CE2	2.56	0.40
1:D:315:SER:HB2	1:D:328:THR:CG2	2.52	0.40
1:A:285:CYS:SG	1:A:288:ALA:HB2	2.62	0.40
1:C:364:GLN:NE2	1:C:365:PRO:O	2.55	0.40
1:C:60:ILE:HD12	1:C:206:VAL:HG21	2.04	0.40
1:B:265:ASN:C	1:B:265:ASN:ND2	2.74	0.40
1:A:309:GLN:NE2	1:A:403:VAL:O	2.55	0.40
1:D:264:TRP:HA	1:D:415:ASN:O	2.21	0.40
1:A:357:ALA:HB2	1:A:367:GLY:O	2.22	0.40
1:A:181:SER:O	1:A:187:ASN:ND2	2.54	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	411/413 (100%)	375 (91%)	32 (8%)	4 (1%)	22	12
1	B	411/413 (100%)	377 (92%)	30 (7%)	4 (1%)	22	12
1	C	411/413 (100%)	378 (92%)	29 (7%)	4 (1%)	22	12
1	D	411/413 (100%)	378 (92%)	29 (7%)	4 (1%)	22	12
All	All	1644/1652 (100%)	1508 (92%)	120 (7%)	16 (1%)	22	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	THR
1	B	244	THR
1	C	244	THR
1	D	244	THR
1	A	272	TYR

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Mol	Chain	Res	Type
1	B	272	TYR
1	C	243	ALA
1	C	272	TYR
1	D	243	ALA
1	D	272	TYR
1	A	243	ALA
1	B	243	ALA
1	A	257	HIS
1	B	257	HIS
1	C	257	HIS
1	D	257	HIS

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	341/341 (100%)	318 (93%)	23 (7%)	23	16
1	B	341/341 (100%)	317 (93%)	24 (7%)	21	14
1	C	341/341 (100%)	315 (92%)	26 (8%)	19	12
1	D	341/341 (100%)	316 (93%)	25 (7%)	20	13
All	All	1364/1364 (100%)	1266 (93%)	98 (7%)	21	13

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	85	THR
1	A	92	LEU
1	A	98	LEU
1	A	103	GLN
1	A	139	GLU
1	A	146	ARG
1	A	171	HIS
1	A	172	GLU
1	A	227	LEU
1	A	228	ILE

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Mol	Chain	Res	Type
1	A	265	ASN
1	A	267	ASN
1	A	268	ASN
1	A	276	THR
1	A	364	GLN
1	A	368	THR
1	A	370	ASN
1	A	379	LEU
1	A	399	ASN
1	A	406	ASN
1	A	409	THR
1	A	414	LEU
1	B	44	GLN
1	B	85	THR
1	B	92	LEU
1	B	98	LEU
1	B	103	GLN
1	B	139	GLU
1	B	146	ARG
1	B	171	HIS
1	B	172	GLU
1	B	199	GLN
1	B	227	LEU
1	B	228	ILE
1	B	265	ASN
1	B	267	ASN
1	B	268	ASN
1	B	276	THR
1	B	364	GLN
1	B	368	THR
1	B	370	ASN
1	B	379	LEU
1	B	399	ASN
1	B	406	ASN
1	B	409	THR
1	B	414	LEU
1	C	44	GLN
1	C	85	THR
1	C	92	LEU
1	C	98	LEU
1	C	103	GLN
1	C	139	GLU

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Mol	Chain	Res	Type
1	C	146	ARG
1	C	171	HIS
1	C	172	GLU
1	C	199	GLN
1	C	227	LEU
1	C	228	ILE
1	C	231	LEU
1	C	265	ASN
1	C	267	ASN
1	C	268	ASN
1	C	276	THR
1	C	364	GLN
1	C	368	THR
1	C	370	ASN
1	C	379	LEU
1	C	399	ASN
1	C	404	THR
1	C	406	ASN
1	C	409	THR
1	C	414	LEU
1	D	44	GLN
1	D	85	THR
1	D	92	LEU
1	D	98	LEU
1	D	103	GLN
1	D	139	GLU
1	D	146	ARG
1	D	171	HIS
1	D	172	GLU
1	D	199	GLN
1	D	227	LEU
1	D	228	ILE
1	D	265	ASN
1	D	267	ASN
1	D	268	ASN
1	D	276	THR
1	D	353	LEU
1	D	364	GLN
1	D	368	THR
1	D	370	ASN
1	D	379	LEU
1	D	399	ASN

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Mol	Chain	Res	Type
1	D	406	ASN
1	D	409	THR
1	D	414	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	44	GLN
1	A	47	ASN
1	A	63	ASN
1	A	123	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	254	ASN
1	A	257	HIS
1	A	265	ASN
1	A	268	ASN
1	A	280	ASN
1	A	309	GLN
1	A	323	GLN
1	A	364	GLN
1	A	370	ASN
1	A	376	ASN
1	A	399	ASN
1	A	415	ASN
1	B	43	GLN
1	B	44	GLN
1	B	63	ASN
1	B	123	ASN
1	B	128	ASN
1	B	156	ASN
1	B	157	GLN
1	B	171	HIS
1	B	182	GLN
1	B	187	ASN

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Mol	Chain	Res	Type
1	B	221	GLN
1	B	232	GLN
1	B	254	ASN
1	B	257	HIS
1	B	265	ASN
1	B	268	ASN
1	B	280	ASN
1	B	309	GLN
1	B	323	GLN
1	B	364	GLN
1	B	370	ASN
1	B	376	ASN
1	B	399	ASN
1	B	415	ASN
1	C	43	GLN
1	C	44	GLN
1	C	63	ASN
1	C	123	ASN
1	C	128	ASN
1	C	156	ASN
1	C	157	GLN
1	C	171	HIS
1	C	182	GLN
1	C	187	ASN
1	C	221	GLN
1	C	232	GLN
1	C	254	ASN
1	C	257	HIS
1	C	265	ASN
1	C	268	ASN
1	C	280	ASN
1	C	309	GLN
1	C	323	GLN
1	C	364	GLN
1	C	370	ASN
1	C	376	ASN
1	C	399	ASN
1	C	415	ASN
1	D	43	GLN
1	D	44	GLN
1	D	63	ASN
1	D	128	ASN

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Mol	Chain	Res	Type
1	D	156	ASN
1	D	157	GLN
1	D	171	HIS
1	D	182	GLN
1	D	187	ASN
1	D	221	GLN
1	D	232	GLN
1	D	254	ASN
1	D	256	ASN
1	D	257	HIS
1	D	265	ASN
1	D	268	ASN
1	D	280	ASN
1	D	309	GLN
1	D	323	GLN
1	D	364	GLN
1	D	370	ASN
1	D	376	ASN
1	D	399	ASN
1	D	415	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 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	NDG	A	438	-	15,15,15	1.42	2 (13%)	21,21,21	1.20	2 (9%)
3	MAN	A	439	-	12,12,12	1.54	4 (33%)	17,17,17	1.82	5 (29%)
4	NAG	A	440	-	15,15,15	0.76	0	21,21,21	0.78	0
3	MAN	A	441	-	12,12,12	0.67	0	17,17,17	0.41	0
2	NDG	A	442	-	15,15,15	1.27	2 (13%)	21,21,21	0.76	0
2	NDG	B	538	-	15,15,15	1.15	2 (13%)	21,21,21	1.12	2 (9%)
3	MAN	B	539	-	12,12,12	1.29	0	17,17,17	1.70	5 (29%)
4	NAG	B	540	-	15,15,15	0.98	1 (6%)	21,21,21	0.80	0
3	MAN	B	541	-	12,12,12	0.83	0	17,17,17	0.45	0
2	NDG	B	542	-	15,15,15	1.31	1 (6%)	21,21,21	0.91	1 (4%)
2	NDG	C	638	-	15,15,15	1.61	2 (13%)	21,21,21	1.20	2 (9%)
3	MAN	C	639	-	12,12,12	1.49	3 (25%)	17,17,17	1.90	5 (29%)
4	NAG	C	640	-	15,15,15	0.95	0	21,21,21	0.74	0
3	MAN	C	641	-	12,12,12	0.67	0	17,17,17	0.47	0
2	NDG	C	642	-	15,15,15	1.42	3 (20%)	21,21,21	0.88	2 (9%)
2	NDG	D	738	-	15,15,15	1.44	2 (13%)	21,21,21	1.18	2 (9%)
3	MAN	D	739	-	12,12,12	1.51	3 (25%)	17,17,17	1.84	4 (23%)
4	NAG	D	740	-	15,15,15	1.05	1 (6%)	21,21,21	0.80	0
3	MAN	D	741	-	12,12,12	0.70	0	17,17,17	0.45	0
2	NDG	D	742	-	15,15,15	1.35	3 (20%)	21,21,21	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	A	438	-	-	0/6/26/26	0/1/1/1
3	MAN	A	439	-	-	0/2/22/22	0/1/1/1
4	NAG	A	440	-	-	2/6/26/26	0/1/1/1
3	MAN	A	441	-	-	0/2/22/22	0/1/1/1
2	NDG	A	442	-	-	0/6/26/26	0/1/1/1
2	NDG	B	538	-	-	0/6/26/26	0/1/1/1
3	MAN	B	539	-	-	0/2/22/22	0/1/1/1
4	NAG	B	540	-	-	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	B	541	-	-	0/2/22/22	0/1/1/1
2	NDG	B	542	-	-	0/6/26/26	0/1/1/1
2	NDG	C	638	-	-	0/6/26/26	0/1/1/1
3	MAN	C	639	-	-	0/2/22/22	0/1/1/1
4	NAG	C	640	-	-	2/6/26/26	0/1/1/1
3	MAN	C	641	-	-	0/2/22/22	0/1/1/1
2	NDG	C	642	-	-	0/6/26/26	0/1/1/1
2	NDG	D	738	-	-	0/6/26/26	0/1/1/1
3	MAN	D	739	-	-	0/2/22/22	0/1/1/1
4	NAG	D	740	-	-	2/6/26/26	0/1/1/1
3	MAN	D	741	-	-	0/2/22/22	0/1/1/1
2	NDG	D	742	-	-	0/6/26/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	638	NDG	C1-C2	3.69	1.57	1.53
2	D	738	NDG	C1-C2	3.60	1.57	1.53
2	A	438	NDG	C1-C2	3.39	1.57	1.53
2	C	642	NDG	C3-C2	2.98	1.59	1.53
2	D	738	NDG	C8-C7	2.86	1.56	1.50
2	B	542	NDG	C3-C2	2.81	1.59	1.53
2	C	638	NDG	C8-C7	2.79	1.56	1.50
3	A	439	MAN	O5-C1	2.79	1.48	1.43
3	C	639	MAN	C4-C5	2.73	1.59	1.53
2	A	438	NDG	C8-C7	2.65	1.56	1.50
2	A	442	NDG	C1-C2	2.56	1.56	1.53
3	A	439	MAN	C3-C2	2.49	1.59	1.52
3	A	439	MAN	O5-C5	2.46	1.50	1.44
3	D	739	MAN	O5-C1	2.42	1.47	1.43
2	A	442	NDG	C3-C2	2.38	1.58	1.53
2	B	538	NDG	C1-C2	2.37	1.55	1.53
3	D	739	MAN	C4-C5	2.34	1.58	1.53
2	D	742	NDG	C1-C2	2.32	1.55	1.53
3	C	639	MAN	C3-C2	2.26	1.58	1.52
3	C	639	MAN	O5-C1	2.24	1.47	1.43
2	C	642	NDG	O7-C7	2.19	1.27	1.23
4	D	740	NAG	C8-C7	2.18	1.55	1.50
3	D	739	MAN	O5-C5	2.15	1.49	1.44
3	A	439	MAN	C4-C5	2.13	1.57	1.53
2	D	742	NDG	C8-C7	2.13	1.55	1.50
2	C	642	NDG	O-C1	2.12	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	540	NAG	O5-C1	2.12	1.47	1.43
2	B	538	NDG	C8-C7	2.03	1.54	1.50
2	D	742	NDG	C3-C2	2.02	1.57	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	739	MAN	C3-C4-C5	-4.21	102.68	110.20
3	C	639	MAN	C3-C4-C5	-3.95	103.14	110.20
3	A	439	MAN	C3-C4-C5	-3.84	103.34	110.20
3	A	439	MAN	O2-C2-C1	-3.72	101.98	109.89
3	B	539	MAN	C3-C4-C5	-3.71	103.58	110.20
3	C	639	MAN	C6-C5-C4	3.55	121.56	113.00
3	C	639	MAN	O2-C2-C1	-3.52	102.41	109.89
3	D	739	MAN	O2-C2-C1	-3.36	102.74	109.89
2	C	638	NDG	C3-C4-C5	3.30	116.09	110.20
2	A	438	NDG	C3-C4-C5	3.13	115.80	110.20
3	D	739	MAN	C6-C5-C4	3.13	120.56	113.00
2	D	738	NDG	C3-C4-C5	3.11	115.75	110.20
2	B	538	NDG	C3-C4-C5	3.03	115.62	110.20
3	B	539	MAN	O2-C2-C1	-2.99	103.54	109.89
3	C	639	MAN	C4-C3-C2	-2.72	105.80	110.82
3	A	439	MAN	C6-C5-C4	2.69	119.51	113.00
3	B	539	MAN	C6-C5-C4	2.65	119.41	113.00
2	B	538	NDG	C4-C3-C2	2.65	114.21	110.44
2	C	638	NDG	C4-C3-C2	2.44	113.91	110.44
2	B	542	NDG	C1-C2-N2	-2.43	108.02	110.85
2	A	438	NDG	C4-C3-C2	2.38	113.83	110.44
3	D	739	MAN	C4-C3-C2	-2.38	106.42	110.82
2	D	738	NDG	C4-C3-C2	2.37	113.80	110.44
3	B	539	MAN	C4-C3-C2	-2.32	106.52	110.82
3	A	439	MAN	C4-C3-C2	-2.27	106.62	110.82
2	C	642	NDG	O-C1-C2	2.25	111.89	109.61
3	A	439	MAN	O5-C1-C2	-2.10	106.60	109.86
3	B	539	MAN	O5-C1-C2	-2.10	106.61	109.86
3	C	639	MAN	O3-C3-C2	2.05	114.94	110.35
2	C	642	NDG	C1-C2-N2	-2.02	108.50	110.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	540	NAG	O7-C7-N2-C2
4	C	640	NAG	O7-C7-N2-C2
4	D	740	NAG	O7-C7-N2-C2
4	A	440	NAG	O7-C7-N2-C2
4	D	740	NAG	C8-C7-N2-C2
4	A	440	NAG	C8-C7-N2-C2
4	B	540	NAG	C8-C7-N2-C2
4	C	640	NAG	C8-C7-N2-C2

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	413/413 (100%)	0.95	35 (8%)	11 10	22, 34, 47, 61	0
1	B	413/413 (100%)	0.86	34 (8%)	12 11	22, 34, 47, 61	0
1	C	413/413 (100%)	0.86	32 (7%)	13 12	22, 34, 47, 61	0
1	D	413/413 (100%)	0.96	40 (9%)	8 8	22, 34, 47, 61	0
All	All	1652/1652 (100%)	0.91	141 (8%)	11 10	22, 34, 48, 61	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	THR	8.0
1	D	244	THR	7.7
1	B	234	THR	7.5
1	C	244	THR	6.8
1	D	323	GLN	6.5
1	C	238	THR	6.5
1	A	238	THR	5.6
1	C	234	THR	5.6
1	A	437	ASN	5.0
1	A	244	THR	4.8
1	B	241	PRO	4.7
1	B	238	THR	4.5
1	A	47	ASN	4.4
1	D	234	THR	4.3
1	B	281	ILE	4.2
1	C	437	ASN	4.1
1	A	240	THR	3.9
1	D	240	THR	3.9
1	B	244	THR	3.6
1	D	212	ASP	3.5
1	D	238	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	242	SER	3.5
1	B	240	THR	3.4
1	D	243	ALA	3.4
1	D	437	ASN	3.4
1	B	253	LEU	3.3
1	D	377	ALA	3.3
1	B	400	THR	3.3
1	A	241	PRO	3.2
1	D	241	PRO	3.1
1	A	312	VAL	3.1
1	C	172	GLU	3.1
1	A	221	GLN	3.0
1	B	46	ILE	3.0
1	B	62	ARG	3.0
1	D	245	THR	3.0
1	B	251	ILE	3.0
1	C	320	LEU	3.0
1	D	425	ARG	3.0
1	D	103	GLN	3.0
1	C	169	GLN	2.9
1	B	166	ILE	2.9
1	C	241	PRO	2.9
1	D	320	LEU	2.9
1	A	323	GLN	2.8
1	D	221	GLN	2.8
1	C	425	ARG	2.8
1	D	166	ILE	2.7
1	A	103	GLN	2.7
1	C	165	LEU	2.7
1	C	243	ALA	2.7
1	D	400	THR	2.7
1	A	209	ILE	2.7
1	A	427	MET	2.7
1	D	199	GLN	2.7
1	A	212	ASP	2.6
1	B	380	SER	2.6
1	D	216	ARG	2.6
1	C	429	GLY	2.6
1	A	133	THR	2.6
1	C	217	THR	2.6
1	B	375	ASP	2.6
1	B	435	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	240	THR	2.6
1	B	103	GLN	2.6
1	C	281	ILE	2.5
1	D	294	THR	2.5
1	A	281	ILE	2.5
1	B	228	ILE	2.5
1	C	221	GLN	2.5
1	D	196	GLY	2.4
1	B	320	LEU	2.4
1	D	379	LEU	2.4
1	D	217	THR	2.4
1	B	134	ASP	2.4
1	A	217	THR	2.4
1	A	243	ALA	2.4
1	D	47	ASN	2.4
1	A	199	GLN	2.4
1	C	218	ARG	2.4
1	A	213	THR	2.3
1	B	252	ARG	2.3
1	A	295	VAL	2.3
1	B	437	ASN	2.3
1	A	254	ASN	2.3
1	B	235	GLY	2.3
1	A	377	ALA	2.3
1	A	219	PHE	2.3
1	D	85	THR	2.3
1	B	243	ALA	2.3
1	A	322	GLY	2.3
1	C	375	ASP	2.3
1	D	293	ALA	2.3
1	C	228	ILE	2.3
1	B	133	THR	2.3
1	D	56	VAL	2.3
1	A	425	ARG	2.3
1	D	250	ASN	2.3
1	B	373	ARG	2.2
1	D	239	ALA	2.2
1	D	60	ILE	2.2
1	A	248	SER	2.2
1	A	433	LEU	2.2
1	B	216	ARG	2.2
1	D	392	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	410	LEU	2.2
1	C	380	SER	2.2
1	C	199	GLN	2.2
1	C	216	ARG	2.2
1	C	133	THR	2.2
1	C	295	VAL	2.2
1	A	170	TYR	2.1
1	A	235	GLY	2.1
1	C	195	ALA	2.1
1	C	373	ARG	2.1
1	C	25	THR	2.1
1	D	318	ILE	2.1
1	A	400	THR	2.1
1	C	158	THR	2.1
1	D	172	GLU	2.1
1	A	62	ARG	2.1
1	B	110	ASN	2.1
1	D	251	ILE	2.1
1	D	327	ALA	2.1
1	C	212	ASP	2.1
1	B	399	ASN	2.1
1	D	305	THR	2.1
1	B	312	VAL	2.1
1	D	312	VAL	2.1
1	A	218	ARG	2.1
1	A	394	ALA	2.1
1	D	436	ALA	2.1
1	B	359	LYS	2.1
1	B	374	ILE	2.1
1	D	404	THR	2.0
1	C	312	VAL	2.0
1	D	375	ASP	2.0
1	B	31	TYR	2.0
1	C	201	THR	2.0
1	B	84	THR	2.0
1	A	166	ILE	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	B	539	12/12	0.30	27.57	15,19,24,34	0
3	MAN	C	639	12/12	0.24	8.37	15,19,24,34	0
2	NDG	D	742	15/15	0.24	5.78	18,24,34,35	0
2	NDG	B	538	15/15	0.27	4.29	18,24,34,35	0
3	MAN	A	439	12/12	0.27	4.03	15,19,24,34	0
5	HG	C	644	1/1	0.43	3.95	67,67,67,67	0
2	NDG	C	638	15/15	0.23	3.67	18,24,34,35	0
2	NDG	D	738	15/15	0.28	2.79	18,24,34,35	0
2	NDG	A	442	15/15	0.26	2.78	18,24,34,35	0
5	HG	D	744	1/1	0.40	2.15	67,67,67,67	0
2	NDG	C	642	15/15	0.28	1.89	18,24,34,35	0
2	NDG	B	542	15/15	0.22	1.82	18,24,34,35	0
2	NDG	A	438	15/15	0.21	1.79	18,24,34,35	0
4	NAG	C	640	15/15	0.23	1.42	18,24,34,35	0
5	HG	A	444	1/1	0.32	1.28	67,67,67,67	0
3	MAN	D	739	12/12	0.22	0.86	15,19,24,34	0
4	NAG	A	440	15/15	0.21	0.83	18,24,34,35	0
5	HG	B	544	1/1	0.29	0.57	67,67,67,67	0
4	NAG	D	740	15/15	0.20	0.06	18,24,34,35	0
4	NAG	B	540	15/15	0.14	-0.89	18,24,34,35	0
5	HG	B	543	1/1	0.07	-2.29	55,55,55,55	0
5	HG	D	743	1/1	0.03	-3.67	55,55,55,55	0
5	HG	C	643	1/1	0.03	-3.84	55,55,55,55	0
5	HG	A	443	1/1	0.04	-6.48	55,55,55,55	0
3	MAN	B	541	12/12	0.23	-	19,24,34,35	0
3	MAN	D	741	12/12	0.20	-	19,24,34,35	0
3	MAN	C	641	12/12	0.29	-	19,24,34,35	0
3	MAN	A	441	12/12	0.22	-	19,24,34,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.