



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:48 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

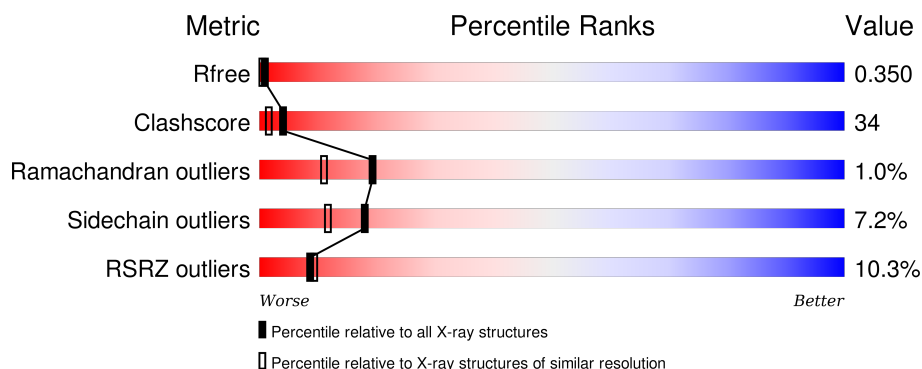
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	413	<div> <div>9%</div> <div>53%</div> <div>42%</div> <div>5%</div> </div>
1	B	413	<div> <div>9%</div> <div>56%</div> <div>39%</div> <div>5%</div> </div>
1	C	413	<div> <div>10%</div> <div>55%</div> <div>39%</div> <div>6%</div> </div>
1	D	413	<div> <div>12%</div> <div>55%</div> <div>40%</div> <div>5%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDG	A	438	-	-	X	X
2	NDG	A	442	-	-	X	X
2	NDG	B	538	-	-	X	X
2	NDG	B	542	-	-	-	X
2	NDG	C	638	-	-	X	X
2	NDG	C	642	-	-	X	-
2	NDG	D	738	-	-	X	X
2	NDG	D	742	-	-	X	X
3	MAN	A	439	-	-	X	-
3	MAN	B	539	-	-	X	-
3	MAN	D	739	-	-	X	-
4	NAG	A	440	-	-	X	-
4	NAG	B	540	-	-	X	-
4	NAG	C	640	-	-	X	-
4	NAG	D	740	-	-	X	-
5	HG	C	644	-	-	-	X
5	HG	D	744	-	-	-	X

2 Entry composition [i](#)

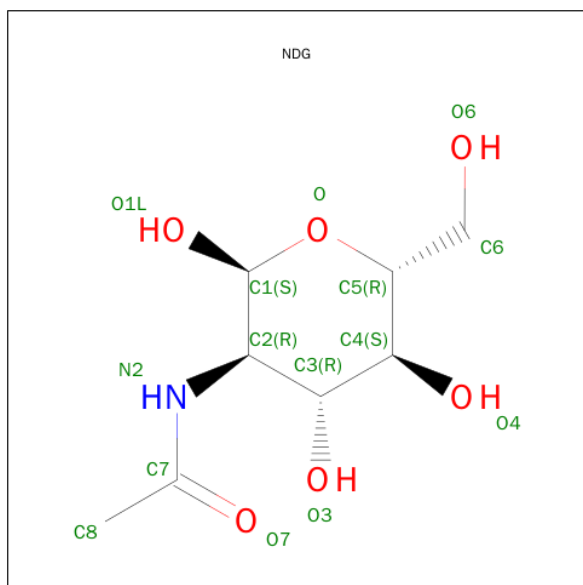
There are 6 unique types of molecules in this entry. The entry contains 13261 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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: $C_8H_{15}NO_6$).



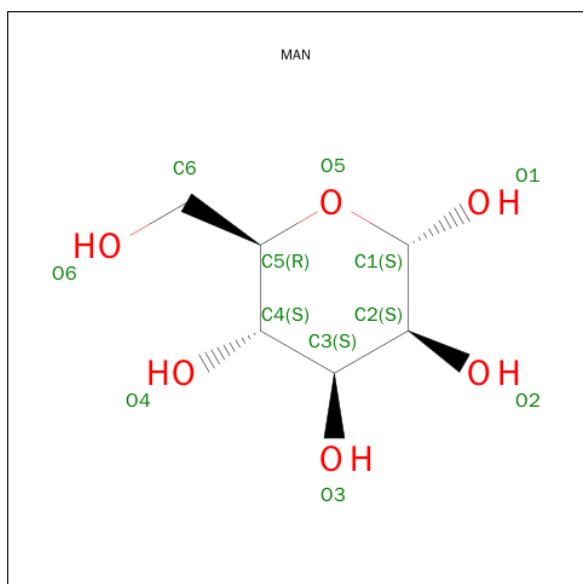
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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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: $C_6H_{12}O_6$).



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

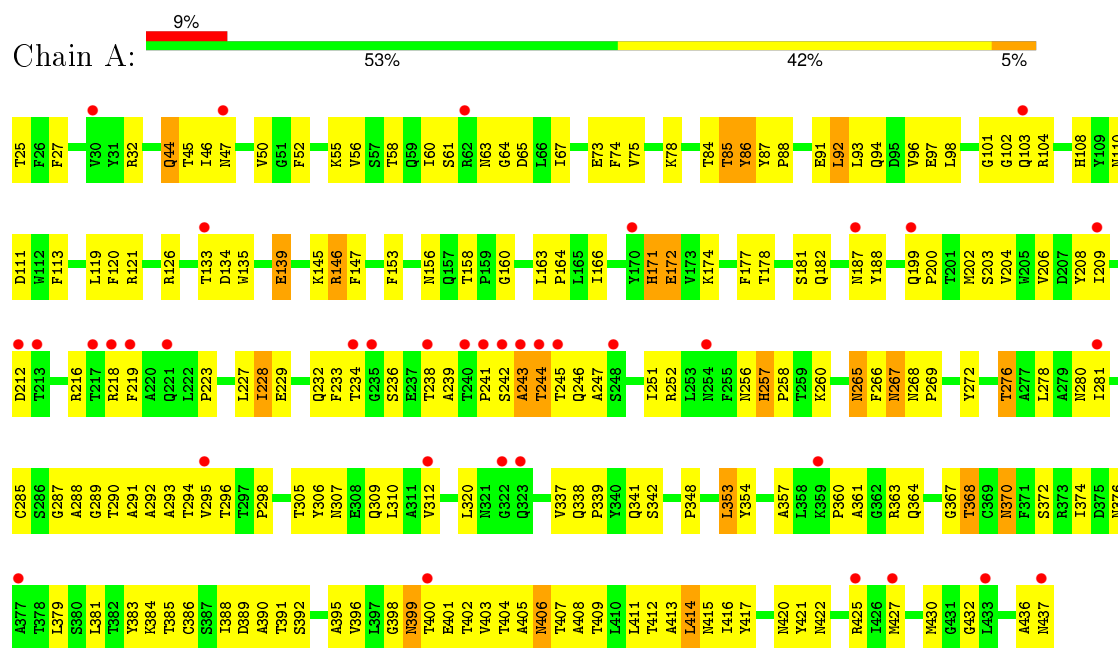
- Molecule 6 is water.

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

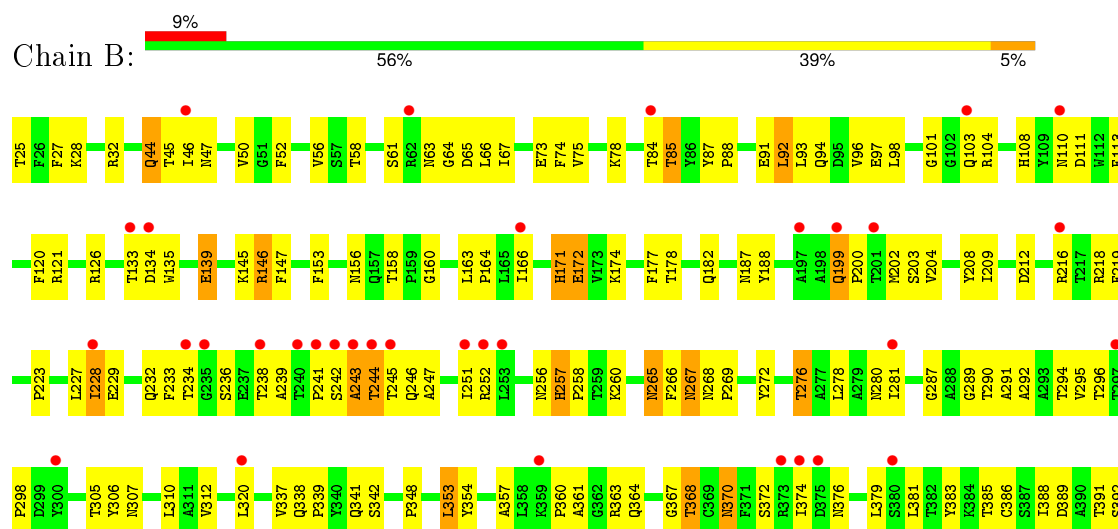
3 Residue-property plots

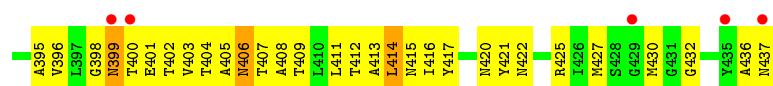
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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

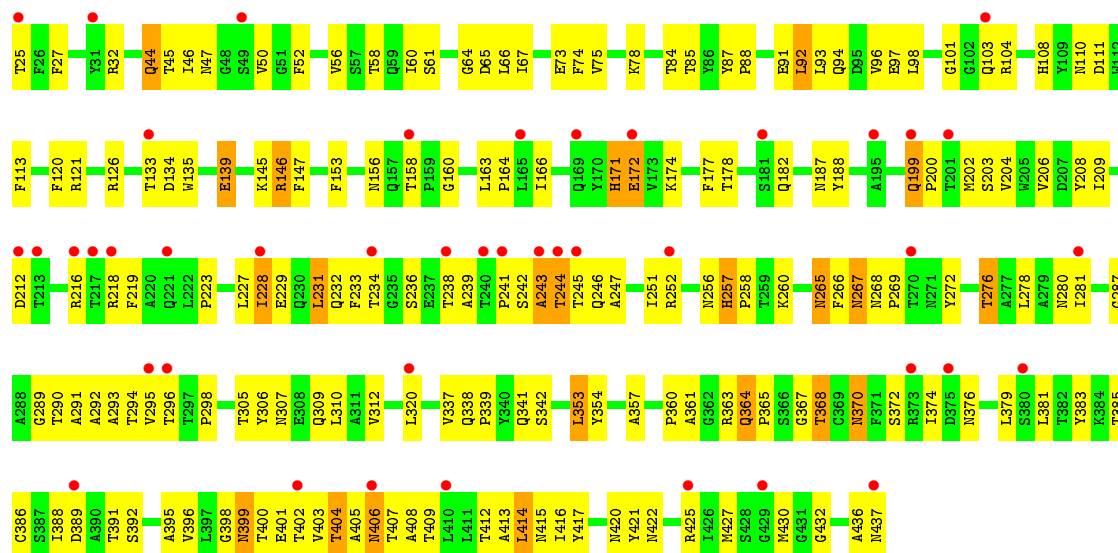


- Molecule 1: The Major capsid protein of PBCV-1, Vp54

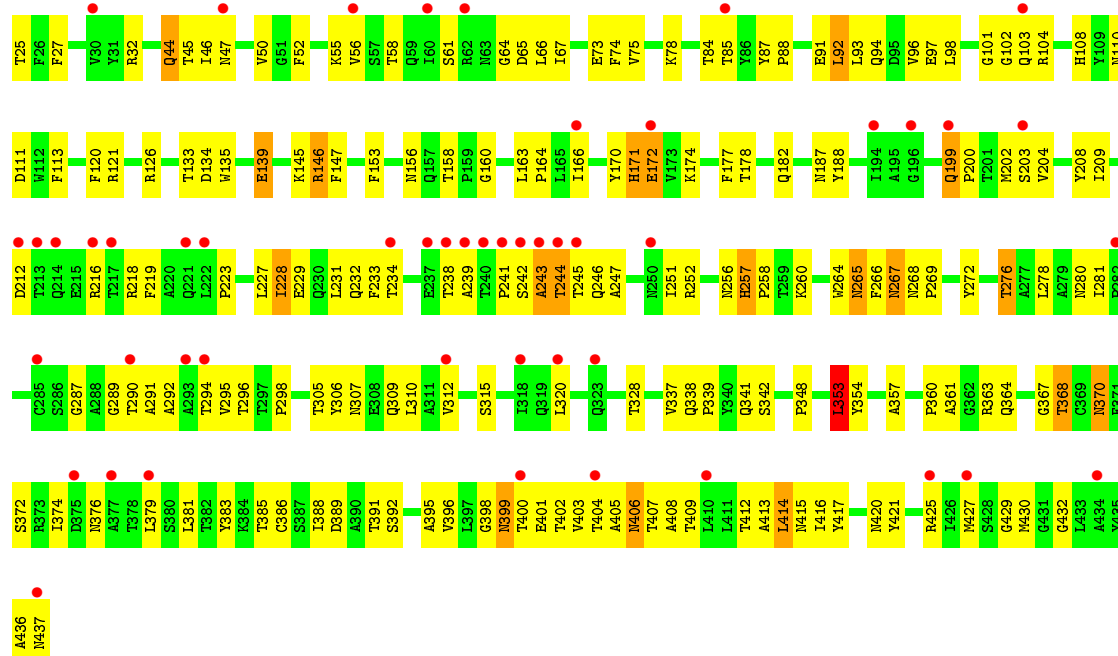




• Molecule 1: The Major capsid protein of PBCV-1, Vp54



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



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 0.342 , 0.350	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)	0.38 , 35.9	EDS
Estimated twinning fraction	0.278 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	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.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts [i](#)

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (887) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:280:ASN:HD21	2:A:438:NDG:C5	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LEU:HD22	1:C:96:VAL:HG22	1.81	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OI1	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
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%)	19	11
1	B	411/413 (100%)	377 (92%)	30 (7%)	4 (1%)	19	11
1	C	411/413 (100%)	378 (92%)	29 (7%)	4 (1%)	19	11
1	D	411/413 (100%)	378 (92%)	29 (7%)	4 (1%)	19	11
All	All	1644/1652 (100%)	1508 (92%)	120 (7%)	16 (1%)	19	11

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
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%)	20	14
1	B	341/341 (100%)	317 (93%)	24 (7%)	19	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	341/341 (100%)	315 (92%)	26 (8%)	16	10
1	D	341/341 (100%)	316 (93%)	25 (7%)	17	11
All	All	1364/1364 (100%)	1266 (93%)	98 (7%)	18	12

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	1.45	2 (13%)	17,21,21	1.30	2 (11%)
3	MAN	A	439	-	12,12,12	1.58	4 (33%)	17,17,17	1.80	5 (29%)
4	NAG	A	440	-	15,15,15	0.78	0	17,21,21	0.84	0
3	MAN	A	441	-	12,12,12	0.70	0	17,17,17	0.40	0
2	NDG	A	442	-	15,15,15	1.30	2 (13%)	17,21,21	0.77	0
2	NDG	B	538	-	15,15,15	1.18	2 (13%)	17,21,21	1.25	2 (11%)
3	MAN	B	539	-	12,12,12	1.31	0	17,17,17	1.68	4 (23%)
4	NAG	B	540	-	15,15,15	1.00	1 (6%)	17,21,21	0.81	0
3	MAN	B	541	-	12,12,12	0.86	0	17,17,17	0.45	0
2	NDG	B	542	-	15,15,15	1.34	1 (6%)	17,21,21	0.70	0
2	NDG	C	638	-	15,15,15	1.65	3 (20%)	17,21,21	1.33	2 (11%)
3	MAN	C	639	-	12,12,12	1.52	3 (25%)	17,17,17	1.88	5 (29%)
4	NAG	C	640	-	15,15,15	0.97	0	17,21,21	0.80	0
3	MAN	C	641	-	12,12,12	0.70	0	17,17,17	0.47	0
2	NDG	C	642	-	15,15,15	1.46	3 (20%)	17,21,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDG	D	738	-	15,15,15	1.47	2 (13%)	17,21,21	1.29	2 (11%)
3	MAN	D	739	-	12,12,12	1.55	3 (25%)	17,17,17	1.82	4 (23%)
4	NAG	D	740	-	15,15,15	1.08	1 (6%)	17,21,21	0.87	0
3	MAN	D	741	-	12,12,12	0.71	0	17,17,17	0.45	0
2	NDG	D	742	-	15,15,15	1.38	3 (20%)	17,21,21	0.65	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
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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	638	NDG	C3-C2	2.00	1.57	1.53
2	C	642	NDG	O7-C7	2.04	1.27	1.23
2	D	742	NDG	C3-C2	2.12	1.57	1.53
2	B	538	NDG	C8-C7	2.14	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	739	MAN	O5-C5	2.16	1.49	1.44
3	A	439	MAN	C4-C5	2.19	1.57	1.53
2	D	742	NDG	C8-C7	2.25	1.55	1.50
4	B	540	NAG	O5-C1	2.25	1.47	1.43
2	C	642	NDG	O-C1	2.25	1.47	1.43
3	C	639	MAN	C3-C2	2.29	1.58	1.52
4	D	740	NAG	C8-C7	2.30	1.55	1.50
2	D	742	NDG	C1-C2	2.33	1.55	1.53
3	C	639	MAN	O5-C1	2.37	1.47	1.43
2	B	538	NDG	C1-C2	2.39	1.55	1.53
3	D	739	MAN	C4-C5	2.40	1.58	1.53
3	A	439	MAN	O5-C5	2.46	1.50	1.44
2	A	442	NDG	C3-C2	2.50	1.58	1.53
3	A	439	MAN	C3-C2	2.52	1.59	1.52
3	D	739	MAN	O5-C1	2.57	1.47	1.43
2	A	442	NDG	C1-C2	2.58	1.56	1.53
2	A	438	NDG	C8-C7	2.79	1.56	1.50
3	C	639	MAN	C4-C5	2.81	1.59	1.53
2	C	638	NDG	C8-C7	2.94	1.56	1.50
3	A	439	MAN	O5-C1	2.95	1.48	1.43
2	B	542	NDG	C3-C2	2.95	1.59	1.53
2	D	738	NDG	C8-C7	3.01	1.56	1.50
2	C	642	NDG	C3-C2	3.13	1.59	1.53
2	A	438	NDG	C1-C2	3.43	1.57	1.53
2	D	738	NDG	C1-C2	3.65	1.57	1.53
2	C	638	NDG	C1-C2	3.74	1.57	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	739	MAN	C3-C4-C5	-4.31	102.68	110.20
3	C	639	MAN	C3-C4-C5	-4.05	103.14	110.20
3	A	439	MAN	C3-C4-C5	-3.93	103.34	110.20
3	B	539	MAN	C3-C4-C5	-3.80	103.58	110.20
3	A	439	MAN	O2-C2-C1	-3.56	101.98	109.82
3	C	639	MAN	O2-C2-C1	-3.36	102.41	109.82
3	D	739	MAN	O2-C2-C1	-3.21	102.74	109.82
3	B	539	MAN	O2-C2-C1	-2.85	103.54	109.82
3	C	639	MAN	C4-C3-C2	-2.68	105.80	110.79
3	D	739	MAN	C4-C3-C2	-2.34	106.42	110.79
3	B	539	MAN	C4-C3-C2	-2.29	106.52	110.79
3	A	439	MAN	C4-C3-C2	-2.23	106.62	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	439	MAN	O5-C1-C2	-2.00	106.60	109.80
3	C	639	MAN	O3-C3-C2	2.05	114.94	110.34
2	D	738	NDG	C4-C3-C2	2.43	113.80	110.43
2	A	438	NDG	C4-C3-C2	2.45	113.83	110.43
2	C	638	NDG	C4-C3-C2	2.51	113.91	110.43
3	B	539	MAN	C6-C5-C4	2.59	119.41	113.02
3	A	439	MAN	C6-C5-C4	2.63	119.51	113.02
2	B	538	NDG	C4-C3-C2	2.72	114.21	110.43
3	D	739	MAN	C6-C5-C4	3.06	120.56	113.02
2	B	538	NDG	C3-C4-C5	3.11	115.62	110.20
2	D	738	NDG	C3-C4-C5	3.19	115.75	110.20
2	A	438	NDG	C3-C4-C5	3.21	115.80	110.20
2	C	638	NDG	C3-C4-C5	3.38	116.09	110.20
3	C	639	MAN	C6-C5-C4	3.47	121.56	113.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

20 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	438	NDG	15	0
3	A	439	MAN	6	0
4	A	440	NAG	15	0
3	A	441	MAN	4	0
2	A	442	NDG	7	0
2	B	538	NDG	12	0
3	B	539	MAN	7	0
4	B	540	NAG	14	0
3	B	541	MAN	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	542	NDG	6	0
2	C	638	NDG	15	0
3	C	639	MAN	5	0
4	C	640	NAG	14	0
3	C	641	MAN	4	0
2	C	642	NDG	7	0
2	D	738	NDG	16	0
3	D	739	MAN	7	0
4	D	740	NAG	16	0
3	D	741	MAN	4	0
2	D	742	NDG	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	413/413 (100%)	0.89	38 (9%)	11 12	22, 34, 47, 61	0
1	B	413/413 (100%)	0.83	39 (9%)	11 11	22, 34, 47, 61	0
1	C	413/413 (100%)	0.85	43 (10%)	8 9	22, 34, 47, 61	0
1	D	413/413 (100%)	0.95	50 (12%)	6 6	22, 34, 47, 61	0
All	All	1652/1652 (100%)	0.88	170 (10%)	9 9	22, 34, 48, 61	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	THR	9.1
1	A	234	THR	9.1
1	B	234	THR	8.2
1	C	244	THR	8.0
1	D	323	GLN	7.6
1	C	238	THR	6.8
1	A	244	THR	6.1
1	B	241	PRO	6.0
1	C	234	THR	6.0
1	A	238	THR	5.7
1	A	437	ASN	5.2
1	D	234	THR	4.9
1	B	244	THR	4.8
1	D	212	ASP	4.5
1	A	47	ASN	4.5
1	B	238	THR	4.5
1	D	240	THR	4.5
1	C	437	ASN	4.5
1	B	281	ILE	4.4
1	B	242	SER	4.3
1	D	243	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	241	PRO	4.2
1	A	240	THR	4.1
1	A	241	PRO	3.9
1	D	245	THR	3.8
1	C	241	PRO	3.8
1	B	240	THR	3.7
1	D	437	ASN	3.6
1	A	212	ASP	3.6
1	D	238	THR	3.6
1	B	253	LEU	3.5
1	B	400	THR	3.4
1	A	323	GLN	3.4
1	D	425	ARG	3.4
1	A	213	THR	3.4
1	D	377	ALA	3.3
1	C	172	GLU	3.3
1	A	243	ALA	3.3
1	C	169	GLN	3.3
1	A	221	GLN	3.3
1	B	166	ILE	3.3
1	C	243	ALA	3.3
1	C	425	ARG	3.3
1	B	46	ILE	3.2
1	D	320	LEU	3.2
1	D	217	THR	3.2
1	D	103	GLN	3.2
1	C	320	LEU	3.1
1	A	427	MET	3.1
1	B	62	ARG	3.1
1	B	375	ASP	3.1
1	A	312	VAL	3.0
1	D	221	GLN	3.0
1	C	375	ASP	3.0
1	D	166	ILE	2.9
1	D	199	GLN	2.9
1	A	217	THR	2.9
1	C	240	THR	2.9
1	B	103	GLN	2.9
1	D	213	THR	2.9
1	B	380	SER	2.8
1	D	196	GLY	2.8
1	C	245	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	221	GLN	2.8
1	A	103	GLN	2.8
1	D	216	ARG	2.8
1	B	243	ALA	2.7
1	B	373	ARG	2.7
1	A	133	THR	2.7
1	C	217	THR	2.7
1	B	251	ILE	2.7
1	C	429	GLY	2.7
1	A	242	SER	2.7
1	D	294	THR	2.7
1	D	47	ASN	2.7
1	C	281	ILE	2.6
1	A	322	GLY	2.6
1	A	209	ILE	2.6
1	A	248	SER	2.6
1	D	400	THR	2.6
1	C	165	LEU	2.6
1	B	435	TYR	2.6
1	A	62	ARG	2.6
1	C	212	ASP	2.6
1	A	199	GLN	2.5
1	A	425	ARG	2.5
1	D	375	ASP	2.5
1	B	252	ARG	2.5
1	C	218	ARG	2.5
1	D	379	LEU	2.5
1	B	134	ASP	2.5
1	B	228	ILE	2.5
1	C	389	ASP	2.5
1	C	228	ILE	2.5
1	D	404	THR	2.5
1	D	250	ASN	2.5
1	C	380	SER	2.5
1	D	172	GLU	2.4
1	C	216	ARG	2.4
1	A	245	THR	2.4
1	D	85	THR	2.4
1	B	437	ASN	2.4
1	C	213	THR	2.4
1	C	373	ARG	2.4
1	D	242	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	216	ARG	2.4
1	B	235	GLY	2.4
1	D	239	ALA	2.4
1	C	406	ASN	2.4
1	A	218	ARG	2.3
1	C	199	GLN	2.3
1	A	235	GLY	2.3
1	A	254	ASN	2.3
1	D	214	GLN	2.3
1	D	290	THR	2.3
1	B	320	LEU	2.3
1	A	281	ILE	2.3
1	B	133	THR	2.3
1	A	219	PHE	2.2
1	B	245	THR	2.2
1	C	133	THR	2.2
1	A	400	THR	2.2
1	C	25	THR	2.2
1	C	402	THR	2.2
1	B	300	TYR	2.2
1	D	318	ILE	2.2
1	C	270	THR	2.2
1	C	49	SER	2.2
1	C	181	SER	2.2
1	D	312	VAL	2.2
1	A	359	LYS	2.2
1	C	195	ALA	2.2
1	B	84	THR	2.1
1	A	295	VAL	2.1
1	C	295	VAL	2.1
1	D	203	SER	2.1
1	A	433	LEU	2.1
1	D	222	LEU	2.1
1	D	427	MET	2.1
1	C	296	THR	2.1
1	D	410	LEU	2.1
1	D	285	CYS	2.1
1	D	293	ALA	2.1
1	A	170	TYR	2.1
1	D	30	VAL	2.1
1	B	399	ASN	2.1
1	B	199	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	187	ASN	2.1
1	D	62	ARG	2.1
1	B	201	THR	2.1
1	C	201	THR	2.1
1	D	194	ILE	2.1
1	C	410	LEU	2.1
1	A	377	ALA	2.1
1	B	297	THR	2.0
1	C	158	THR	2.0
1	B	374	ILE	2.0
1	B	359	LYS	2.0
1	B	429	GLY	2.0
1	B	197	ALA	2.0
1	D	237	GLU	2.0
1	D	56	VAL	2.0
1	C	252	ARG	2.0
1	C	103	GLN	2.0
1	D	434	ALA	2.0
1	B	110	ASN	2.0
1	A	30	VAL	2.0
1	C	31	TYR	2.0
1	D	282	PRO	2.0
1	D	60	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NDG	D	742	15/15	0.67	0.27	7.75	18,24,34,35	0
2	NDG	B	538	15/15	0.57	0.28	4.91	18,24,34,35	0
5	HG	C	644	1/1	0.89	0.48	4.36	67,67,67,67	0
2	NDG	D	738	15/15	0.54	0.29	3.70	18,24,34,35	0
2	NDG	C	638	15/15	0.64	0.25	3.54	18,24,34,35	0
2	NDG	B	542	15/15	0.68	0.25	3.21	18,24,34,35	0
2	NDG	A	442	15/15	0.68	0.29	2.87	18,24,34,35	0
5	HG	D	744	1/1	0.89	0.45	2.45	67,67,67,67	0
2	NDG	A	438	15/15	0.67	0.21	2.17	18,24,34,35	0
2	NDG	C	642	15/15	0.61	0.32	1.94	18,24,34,35	0
5	HG	A	444	1/1	0.88	0.37	1.74	67,67,67,67	0
4	NAG	C	640	15/15	0.69	0.24	1.30	18,24,34,35	0
4	NAG	A	440	15/15	0.79	0.21	0.92	18,24,34,35	0
4	NAG	D	740	15/15	0.77	0.21	0.87	18,24,34,35	0
5	HG	B	544	1/1	0.93	0.35	0.87	67,67,67,67	0
4	NAG	B	540	15/15	0.80	0.15	-0.65	18,24,34,35	0
5	HG	B	543	1/1	0.97	0.12	-1.25	55,55,55,55	0
5	HG	D	743	1/1	0.97	0.06	-2.91	55,55,55,55	0
5	HG	C	643	1/1	0.98	0.05	-3.67	55,55,55,55	0
5	HG	A	443	1/1	0.96	0.06	-5.32	55,55,55,55	0
3	MAN	C	639	12/12	0.67	0.27	-	15,19,24,34	0
3	MAN	B	541	12/12	0.61	0.26	-	19,24,34,35	0
3	MAN	D	741	12/12	0.74	0.23	-	19,24,34,35	0
3	MAN	A	441	12/12	0.66	0.25	-	19,24,34,35	0
3	MAN	B	539	12/12	0.54	0.34	-	15,19,24,34	0
3	MAN	D	739	12/12	0.56	0.25	-	15,19,24,34	0
3	MAN	A	439	12/12	0.48	0.29	-	15,19,24,34	0
3	MAN	C	641	12/12	0.64	0.32	-	19,24,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.