



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 09:40 PM EDT

PDB ID : 3QHM
Title : Crystal analysis of the complex structure, E342A-cellobiotetraose, of endocellulase from *pyrococcus horikoshii*
Authors : Kim, H.-W.; Ishikawa, K.
Deposited on : unknown
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

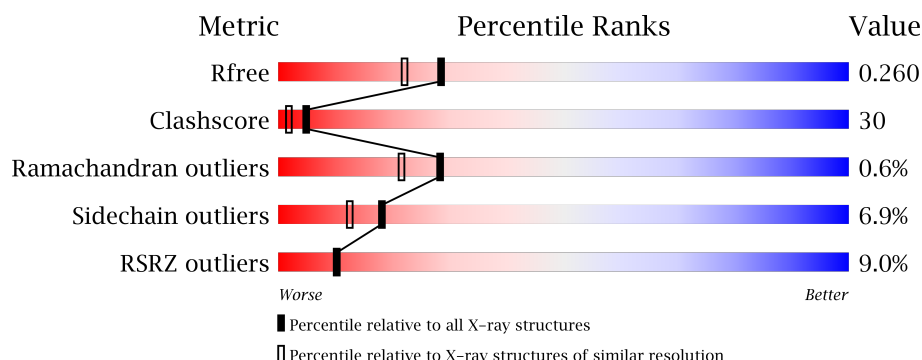
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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	458	<div> <div>8%</div> <div>40%</div> <div>34%</div> <div>6%</div> <div>18%</div> </div>
1	B	458	<div> <div>2%</div> <div>68%</div> <div>13%</div> <div>1%</div> <div>18%</div> </div>
1	C	458	<div> <div>12%</div> <div>48%</div> <div>32%</div> <div>1%</div> <div>18%</div> </div>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9565 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.

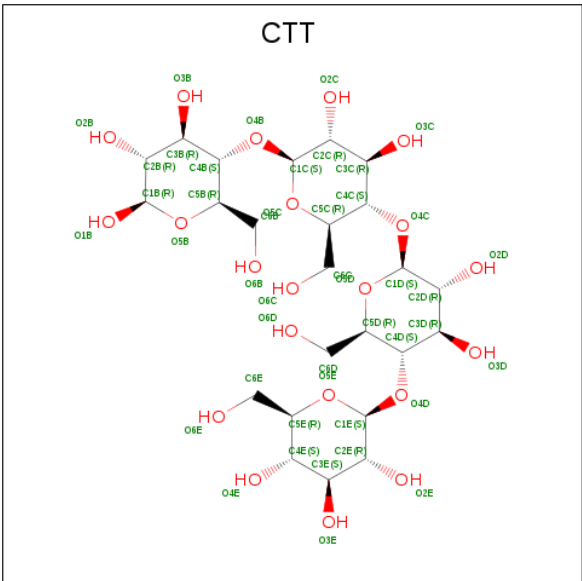
- Molecule 1 is a protein called 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			
1	B	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			
1	C	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			

There are 3 discrepancies between the modelled and reference sequences:

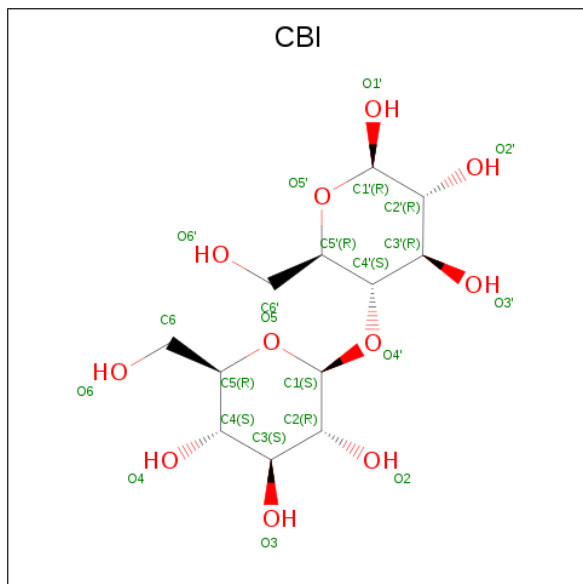
Chain	Residue	Modelled	Actual	Comment	Reference
A	342	ALA	GLU	ENGINEERED MUTATION	UNP O58925
B	342	ALA	GLU	ENGINEERED MUTATION	UNP O58925
C	342	ALA	GLU	ENGINEERED MUTATION	UNP O58925

- Molecule 2 is beta-D-glucopyranosyl-(1->4)-beta-D-glucopyranosyl-(1->4)-beta-D-glucopyranosyl-(1->4)-beta-D-glucopyranose (three-letter code: CTT) (formula: C₂₄H₄₂O₂₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			45	24	21		
2	B	1	Total	C	O	0	0
			45	24	21		
2	C	1	Total	C	O	0	0
			45	24	21		

- Molecule 3 is CELLOBIOSE (three-letter code: CBI) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			23	12	11		

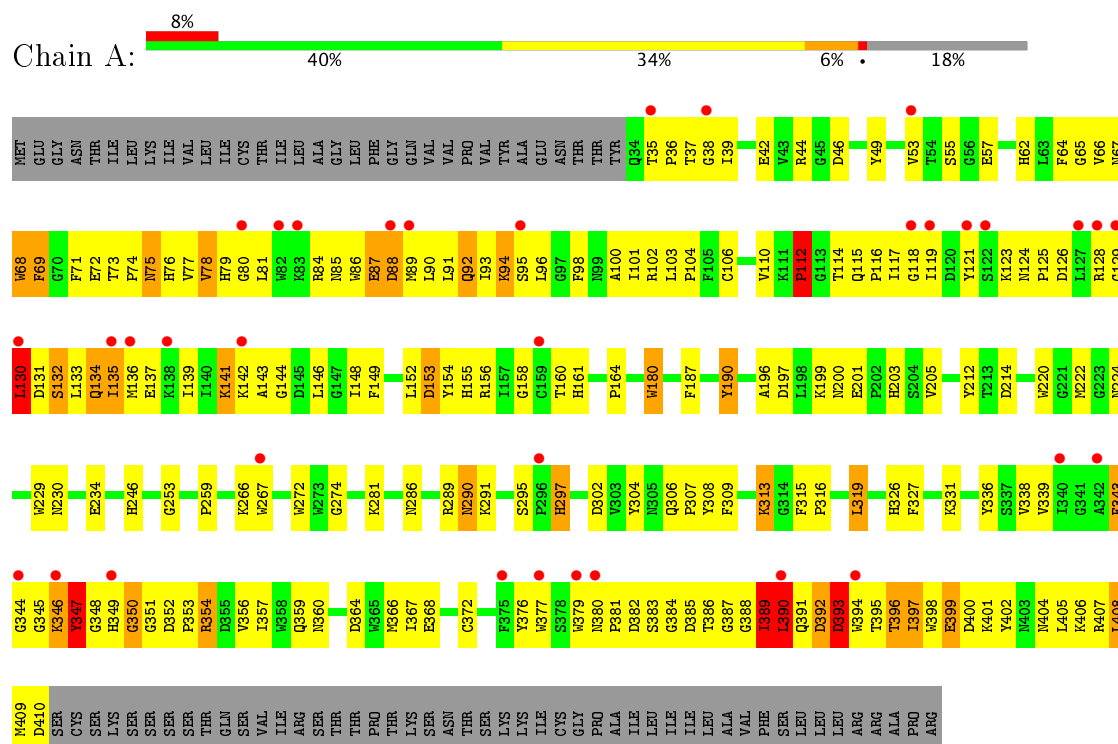
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	97	Total	O	0	0
			97	97		
4	C	42	Total	O	0	0
			42	42		

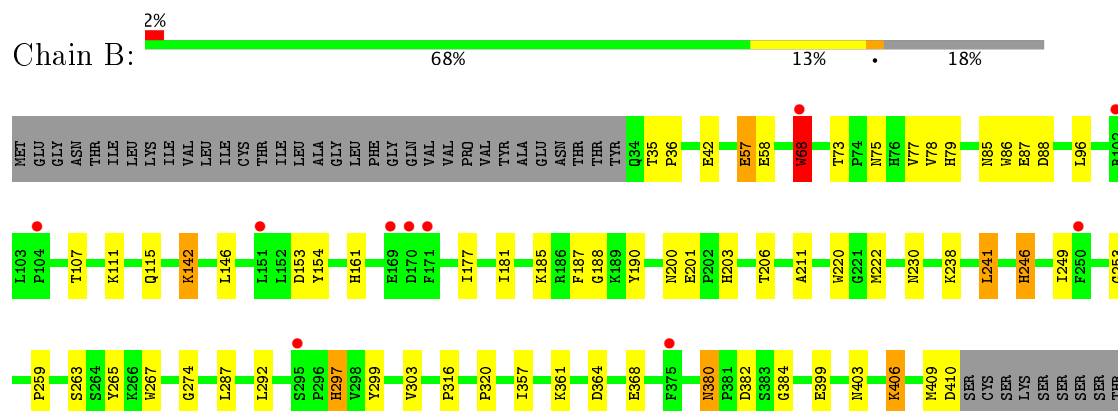
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: 458aa long hypothetical endo-1,4-beta-glucanase

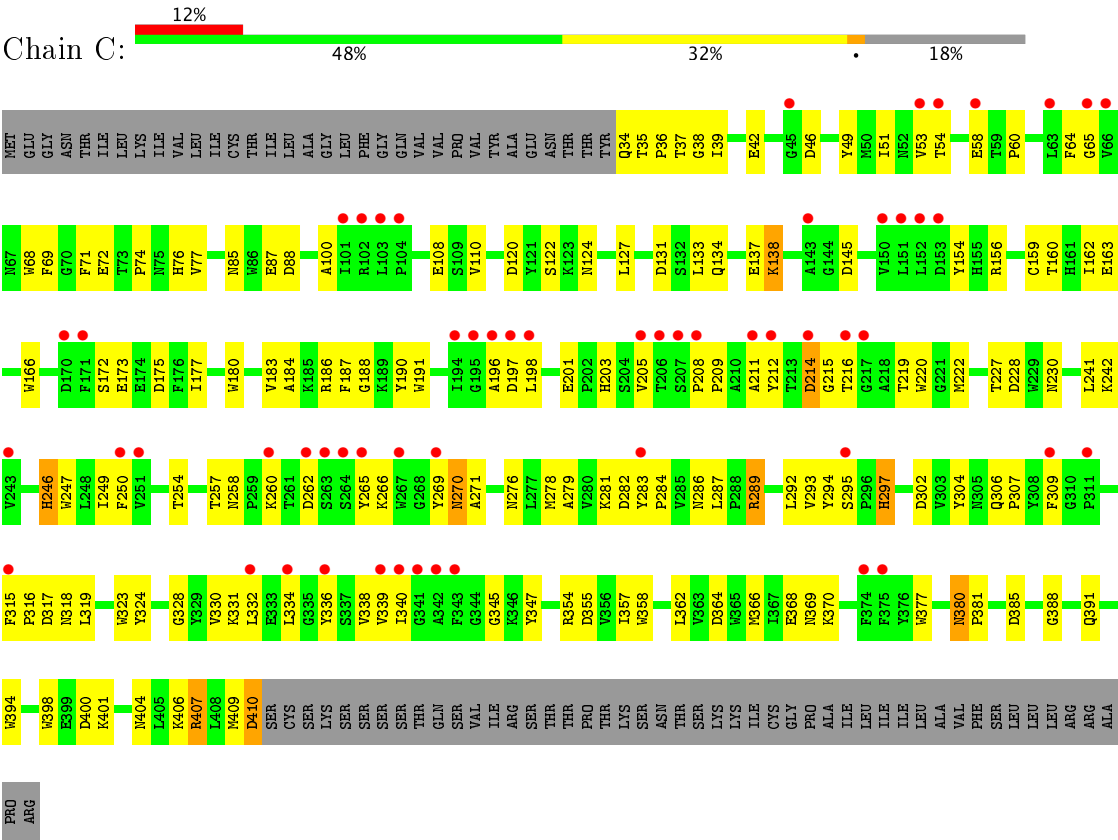


- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



GLN	SER	VAL	ILE	ARG	SER	THR	THR	PRO	THR	LYS	SER	ASN	THR	SER	LYS	LYS	ILE	ILE	CYS	GLY	PRO	GLY	ALA	ILE	ILE	LEU	ILE	ILE	LEU	ALA	VAL	PHE	SER	THR	LEU	LEU	ARG	ARG	ALA	PRO	ARG
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- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.53Å 58.60Å 139.06Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	35.25 – 2.01 35.25 – 2.01	Depositor EDS
% Data completeness (in resolution range)	87.7 (35.25-2.01) 87.5 (35.25-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.261 0.227 , 0.260	Depositor DCC
R_{free} test set	3703 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9565	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTT, CBI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/3178	0.81	9/4339 (0.2%)
1	B	0.38	0/3178	0.69	1/4339 (0.0%)
1	C	0.32	0/3178	0.65	0/4339
All	All	0.37	0/9534	0.72	10/13017 (0.1%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	TYR	N-CA-C	-8.56	87.89	111.00
1	A	393	ASP	N-CA-C	-8.50	88.06	111.00
1	A	130	LEU	CA-CB-CG	7.18	131.81	115.30
1	A	348	GLY	N-CA-C	6.17	128.53	113.10
1	A	130	LEU	N-CA-C	6.05	127.34	111.00
1	B	68	TRP	CA-CB-CG	5.86	124.83	113.70
1	A	347	TYR	CA-CB-CG	5.67	124.16	113.40
1	A	115	GLN	C-N-CD	5.49	139.94	128.40
1	A	389	ILE	N-CA-C	-5.37	96.51	111.00
1	A	197	ASP	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	TYR	Sidechain

5.2 Too-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 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	3067	0	2909	330	1
1	B	3067	0	2909	67	0
1	C	3067	0	2909	157	0
2	A	45	0	41	3	0
2	B	45	0	42	0	0
2	C	45	0	42	2	0
3	C	23	0	22	2	0
4	A	67	0	0	18	0
4	B	97	0	0	10	2
4	C	42	0	0	5	2
All	All	9565	0	8874	551	3

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 30.

All (551) 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)
1:A:381:PRO:HA	1:A:388:GLY:H	1.10	1.12
1:A:389:ILE:HD13	1:A:401:LYS:HE3	1.31	1.10
1:A:76:HIS:CD2	1:A:114:THR:HG21	1.90	1.05
1:A:402:TYR:HA	4:A:515:HOH:O	1.58	1.02
1:A:131:ASP:O	1:A:133:LEU:N	1.93	1.01
1:A:75:ASN:ND2	1:A:75:ASN:H	1.58	1.00
1:A:131:ASP:OD2	1:A:134:GLN:CG	2.11	0.99
1:A:112:PRO:O	1:A:131:ASP:HB3	1.62	0.99
1:A:131:ASP:OD2	1:A:134:GLN:HG2	1.62	0.99
1:A:87:GLU:HA	1:A:90:LEU:HD13	1.45	0.98
1:A:389:ILE:CD1	1:A:401:LYS:HE3	1.93	0.97
1:A:130:LEU:HB2	1:A:134:GLN:HG3	1.46	0.97
1:A:75:ASN:H	1:A:75:ASN:HD22	1.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:O	1:A:137:GLU:HG3	1.66	0.95
1:C:211:ALA:HA	1:C:216:THR:HG21	1.51	0.92
1:A:119:ILE:HG13	1:A:121:TYR:CE1	2.05	0.92
1:A:347:TYR:OH	1:A:360:ASN:CG	2.08	0.92
1:A:131:ASP:OD2	1:A:134:GLN:CD	2.10	0.91
1:A:390:LEU:HA	1:A:397:ILE:HA	1.53	0.90
1:B:380:ASN:HD22	1:B:380:ASN:H	1.18	0.89
1:A:131:ASP:C	1:A:133:LEU:H	1.76	0.88
1:A:381:PRO:HA	1:A:388:GLY:N	1.87	0.88
1:A:88:ASP:O	1:A:92:GLN:HB2	1.74	0.88
1:A:85:ASN:HD21	1:A:87:GLU:HG2	1.39	0.87
1:A:91:LEU:HA	4:A:513:HOH:O	1.72	0.87
1:A:77:VAL:HG23	1:A:116:PRO:HB3	1.56	0.86
1:A:68:TRP:CE2	1:A:78:VAL:HG11	2.11	0.86
1:A:75:ASN:N	1:A:75:ASN:HD22	1.75	0.85
1:A:146:LEU:HD11	4:A:473:HOH:O	1.76	0.85
1:C:201:GLU:OE2	1:C:297:HIS:HD2	1.58	0.85
1:C:318:ASN:OD1	1:C:319:LEU:HD12	1.75	0.85
1:C:269:TYR:C	1:C:270:ASN:HD22	1.80	0.83
1:A:224:ASN:HD21	1:B:75:ASN:HD21	1.27	0.83
1:A:78:VAL:HG12	4:A:502:HOH:O	1.80	0.82
1:C:198:LEU:HD21	1:C:249:ILE:CG2	2.10	0.82
1:B:146:LEU:HG	4:B:532:HOH:O	1.77	0.82
1:A:389:ILE:CG2	1:A:389:ILE:O	2.27	0.82
1:A:81:LEU:O	1:A:81:LEU:HD23	1.79	0.81
1:C:198:LEU:HD21	1:C:249:ILE:HG23	1.60	0.81
1:A:68:TRP:CZ2	1:A:78:VAL:HG11	2.15	0.81
1:A:364:ASP:O	1:A:368:GLU:HG3	1.81	0.81
1:A:131:ASP:O	1:A:134:GLN:N	2.14	0.80
1:B:384:GLY:HA3	4:B:524:HOH:O	1.81	0.80
1:C:85:ASN:HD22	1:C:88:ASP:H	1.29	0.80
1:C:214:ASP:OD1	1:C:216:THR:HB	1.82	0.80
1:C:254:THR:O	1:C:276:ASN:HB3	1.81	0.79
1:A:266:LYS:HE2	1:A:267:TRP:NE1	1.98	0.79
1:C:205:VAL:HG22	1:C:216:THR:O	1.83	0.78
1:C:270:ASN:N	1:C:270:ASN:HD22	1.80	0.78
1:A:85:ASN:HA	1:A:124:ASN:HD21	1.50	0.77
1:A:315:PHE:CE2	1:A:354:ARG:HG2	2.20	0.77
1:A:393:ASP:OD2	1:A:396:THR:HG22	1.85	0.77
1:C:64:PHE:HB3	1:C:409:MET:HE3	1.66	0.76
1:A:290:ASN:HD22	1:A:290:ASN:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLY:C	1:A:130:LEU:HD22	2.06	0.76
1:C:35:THR:HG22	1:C:38:GLY:H	1.49	0.76
1:C:35:THR:HG22	1:C:37:THR:H	1.51	0.75
1:A:381:PRO:HD2	1:A:394:TRP:CH2	2.20	0.75
1:A:347:TYR:CD1	1:A:356:VAL:HA	2.22	0.74
1:A:389:ILE:HG22	1:A:389:ILE:O	1.87	0.74
1:C:124:ASN:HB3	1:C:127:LEU:HD12	1.69	0.74
1:A:71:PHE:HB2	1:A:104:PRO:O	1.87	0.74
1:A:81:LEU:HD22	1:A:119:ILE:HB	1.70	0.74
1:A:190:TYR:HD2	1:A:190:TYR:N	1.85	0.74
1:A:347:TYR:OH	1:A:360:ASN:OD1	2.04	0.74
1:A:214:ASP:HB3	4:B:524:HOH:O	1.86	0.74
1:A:37:THR:HG22	1:A:39:ILE:H	1.53	0.74
1:A:75:ASN:HA	1:A:117:ILE:HB	1.70	0.74
1:B:253:GLY:O	1:B:274:GLY:HA2	1.87	0.74
1:A:381:PRO:HD2	1:A:394:TRP:CZ2	2.24	0.73
1:A:73:THR:HB	1:A:74:PRO:HD2	1.69	0.73
1:A:71:PHE:HZ	1:A:135:ILE:HD11	1.52	0.73
1:A:89:MET:O	1:A:93:ILE:HG12	1.89	0.72
1:A:190:TYR:CD2	1:A:190:TYR:N	2.56	0.72
1:A:406:LYS:HA	1:A:409:MET:CE	2.19	0.72
1:C:306:GLN:OE1	1:C:307:PRO:HD2	1.88	0.72
1:A:144:GLY:HA3	4:A:501:HOH:O	1.88	0.72
1:A:112:PRO:O	1:A:131:ASP:CB	2.37	0.72
1:C:35:THR:HG21	1:C:39:ILE:O	1.90	0.72
1:A:75:ASN:ND2	1:A:75:ASN:N	2.34	0.71
1:A:81:LEU:HB2	4:A:502:HOH:O	1.89	0.71
1:C:214:ASP:C	1:C:216:THR:H	1.93	0.71
1:A:76:HIS:O	1:A:132:SER:HB3	1.89	0.71
1:A:76:HIS:CD2	1:A:114:THR:CG2	2.71	0.71
1:C:214:ASP:O	1:C:216:THR:N	2.19	0.71
1:B:380:ASN:N	1:B:380:ASN:HD22	1.89	0.71
1:B:241:LEU:HD13	1:B:249:ILE:HD11	1.74	0.70
1:C:35:THR:CG2	1:C:38:GLY:H	2.05	0.70
1:C:35:THR:HG22	1:C:37:THR:N	2.06	0.70
1:A:349:HIS:C	1:A:351:GLY:N	2.42	0.70
1:A:407:ARG:O	1:A:410:ASP:HB3	1.92	0.69
1:A:347:TYR:CD2	1:A:356:VAL:HG13	2.28	0.69
1:C:201:GLU:OE2	1:C:297:HIS:CD2	2.44	0.69
1:A:345:GLY:O	1:A:346:LYS:HG3	1.92	0.68
1:A:86:TRP:O	1:A:89:MET:HB2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HA	1:A:409:MET:HE3	1.76	0.68
1:A:390:LEU:HD23	1:A:391:GLN:H	1.57	0.68
1:A:349:HIS:O	1:A:351:GLY:N	2.26	0.68
1:A:131:ASP:C	1:A:133:LEU:N	2.38	0.67
1:A:87:GLU:HA	1:A:90:LEU:CD1	2.23	0.67
1:A:86:TRP:O	1:A:90:LEU:HD12	1.94	0.67
1:C:391:GLN:HG2	1:C:398:TRP:CE2	2.30	0.67
1:C:330:VAL:HG12	1:C:336:TYR:HB2	1.75	0.67
1:A:68:TRP:HE3	1:A:380:ASN:HD21	1.41	0.66
1:A:199:LYS:HE2	1:A:200:ASN:O	1.94	0.66
1:A:405:LEU:HB3	4:A:515:HOH:O	1.95	0.66
1:A:390:LEU:O	1:A:391:GLN:HG3	1.96	0.66
1:A:68:TRP:CG	1:A:78:VAL:HG21	2.30	0.66
1:C:316:PRO:O	1:C:319:LEU:HD13	1.95	0.66
1:A:349:HIS:C	1:A:351:GLY:H	1.97	0.66
1:A:84:ARG:NH1	1:A:394:TRP:O	2.28	0.66
1:A:91:LEU:HD23	4:A:473:HOH:O	1.94	0.66
1:C:289:ARG:NH1	1:C:336:TYR:CE1	2.64	0.66
1:A:346:LYS:HA	1:A:401:LYS:HG3	1.78	0.66
1:B:201:GLU:OE2	1:B:297:HIS:HD2	1.79	0.66
1:B:403:ASN:HA	1:B:406:LYS:CD	2.26	0.65
1:B:85:ASN:HD22	1:B:88:ASP:H	1.44	0.65
1:A:397:ILE:HG22	4:A:478:HOH:O	1.97	0.65
1:A:93:ILE:HD11	1:A:379:TRP:CD2	2.32	0.65
1:A:71:PHE:CZ	1:A:135:ILE:HD11	2.31	0.64
1:B:246:HIS:CD2	1:B:246:HIS:H	2.15	0.64
1:B:364:ASP:O	1:B:368:GLU:HG3	1.97	0.64
1:A:81:LEU:HD22	1:A:119:ILE:CG2	2.27	0.64
1:A:402:TYR:OH	1:A:406:LYS:NZ	2.31	0.64
1:A:89:MET:HE1	1:A:394:TRP:HE3	1.63	0.64
1:A:84:ARG:HD3	1:A:89:MET:CE	2.28	0.64
1:C:354:ARG:HA	1:C:357:ILE:HD12	1.80	0.64
1:C:380:ASN:H	1:C:380:ASN:HD22	1.46	0.64
1:A:366:MET:HB2	1:A:408:LEU:HD11	1.81	0.63
1:A:85:ASN:ND2	1:A:87:GLU:HG2	2.13	0.63
1:B:403:ASN:HA	1:B:406:LYS:HD3	1.80	0.63
1:C:208:PRO:HA	1:C:211:ALA:H	1.64	0.63
1:A:364:ASP:OD1	1:A:407:ARG:NH2	2.27	0.62
1:A:119:ILE:HG13	1:A:121:TYR:HE1	1.62	0.62
1:C:198:LEU:H	1:C:198:LEU:HD22	1.65	0.62
1:A:85:ASN:HA	1:A:124:ASN:ND2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:HE3	1:A:386:THR:C	2.20	0.62
1:A:77:VAL:HG12	1:A:78:VAL:O	1.99	0.62
1:A:246:HIS:H	1:A:246:HIS:CD2	2.16	0.61
1:A:347:TYR:CE1	1:A:356:VAL:O	2.53	0.61
1:C:306:GLN:HB2	1:C:309:PHE:CE2	2.35	0.61
1:C:246:HIS:H	1:C:246:HIS:CD2	2.17	0.61
1:A:62:HIS:CD2	1:A:372:CYS:SG	2.94	0.61
1:C:49:TYR:CE1	1:C:60:PRO:HG3	2.35	0.61
1:A:81:LEU:HD22	1:A:119:ILE:CB	2.30	0.61
1:B:142:LYS:HE2	1:B:146:LEU:HD11	1.83	0.61
1:C:316:PRO:HG3	1:C:357:ILE:CG2	2.31	0.61
1:A:160:THR:HB	1:A:161:HIS:HD2	1.66	0.60
1:C:76:HIS:NE2	1:C:159:CYS:SG	2.74	0.60
1:C:39:ILE:HD13	1:C:191:TRP:HB2	1.83	0.60
1:A:72:GLU:O	1:A:72:GLU:HG2	2.02	0.60
1:A:89:MET:HE3	1:A:394:TRP:CZ3	2.37	0.60
1:A:392:ASP:O	1:A:394:TRP:N	2.35	0.60
1:C:276:ASN:OD1	1:C:278:MET:HG3	2.01	0.60
1:A:344:GLY:HA3	1:A:377:TRP:O	2.02	0.60
1:A:399:GLU:H	1:A:399:GLU:CD	2.03	0.60
1:B:297:HIS:HE1	4:B:484:HOH:O	1.84	0.60
1:C:137:GLU:OE2	1:C:186:ARG:HD3	2.01	0.60
1:A:80:GLY:HA3	1:A:394:TRP:CE3	2.37	0.59
1:A:55:SER:OG	1:A:57:GLU:HG3	2.02	0.59
1:B:79:HIS:HD2	1:B:382:ASP:OD2	1.85	0.59
1:A:93:ILE:HD13	1:A:379:TRP:CE3	2.38	0.59
1:A:133:LEU:O	1:A:136:MET:HB3	2.03	0.59
1:C:219:THR:HG23	1:C:228:ASP:OD1	2.02	0.59
1:C:306:GLN:HB2	1:C:309:PHE:CD2	2.37	0.59
1:A:383:SER:O	1:A:385:ASP:N	2.36	0.59
1:A:89:MET:HE1	1:A:394:TRP:CE3	2.37	0.59
1:C:271:ALA:CB	1:C:276:ASN:HB2	2.33	0.59
1:A:156:ARG:HB3	1:A:158:GLY:O	2.03	0.58
1:C:163:GLU:HB3	4:C:462:HOH:O	2.01	0.58
1:A:86:TRP:H	1:A:124:ASN:HD21	1.51	0.58
1:A:84:ARG:HD3	1:A:89:MET:SD	2.43	0.58
1:B:96:LEU:O	1:B:409:MET:HE1	2.03	0.58
1:C:319:LEU:H	1:C:319:LEU:HD12	1.67	0.58
1:A:77:VAL:HG23	1:A:116:PRO:CB	2.30	0.58
1:A:84:ARG:HD3	1:A:89:MET:HE1	1.85	0.58
1:C:34:GLN:HG3	1:C:53:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:TYR:O	1:A:125:PRO:HG3	2.03	0.58
1:A:379:TRP:CE3	1:A:389:ILE:HG22	2.39	0.58
1:A:90:LEU:O	1:A:93:ILE:HB	2.02	0.58
1:C:315:PHE:CE1	1:C:316:PRO:HB3	2.39	0.58
1:A:352:ASP:OD2	1:A:353:PRO:N	2.36	0.58
1:A:391:GLN:O	1:A:393:ASP:O	2.21	0.58
1:C:180:TRP:O	1:C:183:VAL:HG22	2.03	0.58
1:A:135:ILE:HG13	1:A:136:MET:N	2.19	0.57
1:A:96:LEU:HD22	1:A:402:TYR:CZ	2.39	0.57
1:A:68:TRP:CE3	1:A:68:TRP:HA	2.39	0.57
1:B:142:LYS:HE2	1:B:146:LEU:CD1	2.34	0.57
1:C:138:LYS:HD2	4:C:471:HOH:O	2.03	0.57
1:C:407:ARG:HH11	1:C:407:ARG:HG2	1.69	0.57
1:C:120:ASP:OD1	1:C:122:SER:HB3	2.04	0.57
1:C:347:TYR:HB2	1:C:401:LYS:HD3	1.86	0.57
1:A:67:ASN:OD1	1:A:102:ARG:HB3	2.05	0.57
1:A:352:ASP:OD2	1:A:354:ARG:N	2.38	0.57
1:A:380:ASN:C	1:A:388:GLY:HA3	2.24	0.57
1:A:400:ASP:OD1	1:A:400:ASP:N	2.38	0.57
1:A:392:ASP:O	1:A:393:ASP:C	2.41	0.57
1:A:391:GLN:OE1	1:A:396:THR:HG23	2.05	0.57
1:B:85:ASN:HD21	1:B:87:GLU:HB3	1.68	0.57
1:A:96:LEU:O	1:A:406:LYS:HE2	2.05	0.57
1:C:219:THR:HG22	1:C:227:THR:C	2.25	0.57
1:A:66:VAL:CG2	1:A:101:ILE:HG22	2.34	0.57
1:C:324:TYR:HA	1:C:328:GLY:HA3	1.87	0.57
1:C:108:GLU:HG3	4:C:493:HOH:O	2.03	0.56
1:A:89:MET:CE	1:A:394:TRP:CE3	2.88	0.56
1:C:380:ASN:N	1:C:380:ASN:HD22	2.03	0.56
1:A:376:TYR:HB3	4:A:517:HOH:O	2.06	0.56
1:A:68:TRP:HE3	1:A:68:TRP:HA	1.71	0.56
1:C:180:TRP:CH2	1:C:196:ALA:HB1	2.41	0.56
1:C:35:THR:CG2	1:C:37:THR:H	2.18	0.56
1:A:72:GLU:HG3	1:A:155:HIS:CD2	2.40	0.56
1:C:297:HIS:HE1	4:C:474:HOH:O	1.89	0.56
1:A:347:TYR:OH	1:A:360:ASN:ND2	2.38	0.56
1:B:403:ASN:O	1:B:406:LYS:HG2	2.06	0.56
1:A:65:GLY:HA2	1:A:100:ALA:O	2.06	0.56
1:A:267:TRP:CZ3	1:A:307:PRO:HG2	2.41	0.56
1:A:359:GLN:NE2	1:A:376:TYR:OH	2.39	0.56
1:A:66:VAL:HG21	1:A:93:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.41	0.56
1:C:209:PRO:HA	1:C:212:TYR:CD2	2.41	0.55
1:A:352:ASP:OD2	1:A:352:ASP:C	2.43	0.55
1:A:80:GLY:HA3	1:A:394:TRP:CD2	2.42	0.55
1:A:66:VAL:HG23	1:A:101:ILE:HG22	1.89	0.55
1:C:270:ASN:N	1:C:270:ASN:ND2	2.53	0.55
1:A:390:LEU:CD2	1:A:391:GLN:H	2.20	0.55
1:A:94:LYS:HB2	1:A:94:LYS:HZ2	1.72	0.55
1:A:93:ILE:CD1	1:A:379:TRP:CD2	2.90	0.54
1:A:404:ASN:O	1:A:407:ARG:HD3	2.06	0.54
1:C:201:GLU:O	1:C:203:HIS:HD2	1.90	0.54
1:B:406:LYS:HB2	1:B:406:LYS:NZ	2.23	0.54
1:A:62:HIS:HD2	1:A:372:CYS:SG	2.30	0.54
1:A:102:ARG:O	1:A:104:PRO:HD3	2.08	0.54
1:A:297:HIS:HE1	4:A:489:HOH:O	1.89	0.54
1:A:406:LYS:HA	1:A:409:MET:HE2	1.89	0.54
1:A:180:TRP:CH2	1:A:196:ALA:HB1	2.43	0.53
1:A:94:LYS:NZ	1:A:146:LEU:HB3	2.23	0.53
1:C:219:THR:OG1	1:C:222:MET:HG2	2.08	0.53
1:C:400:ASP:OD1	1:C:401:LYS:N	2.41	0.53
1:C:404:ASN:O	1:C:407:ARG:HB2	2.08	0.53
1:A:117:ILE:CG2	1:A:118:GLY:N	2.72	0.53
1:A:76:HIS:HB3	1:A:132:SER:OG	2.08	0.53
1:C:409:MET:O	1:C:410:ASP:HB2	2.07	0.53
1:C:364:ASP:O	1:C:368:GLU:HG3	2.08	0.53
1:B:246:HIS:HD2	1:B:246:HIS:H	1.56	0.53
1:A:380:ASN:O	1:A:388:GLY:N	2.42	0.53
1:A:64:PHE:CZ	1:A:409:MET:HA	2.43	0.53
1:A:131:ASP:O	1:A:134:GLN:HG2	2.08	0.53
1:A:346:LYS:HE3	1:A:386:THR:CA	2.39	0.53
1:A:289:ARG:HB2	1:C:145:ASP:HA	1.91	0.52
1:A:161:HIS:HA	4:A:508:HOH:O	2.08	0.52
1:C:35:THR:OG1	1:C:246:HIS:HB3	2.09	0.52
1:A:94:LYS:HD3	4:A:499:HOH:O	2.08	0.52
1:A:135:ILE:HD12	1:A:135:ILE:C	2.30	0.52
1:C:219:THR:CG2	1:C:227:THR:OG1	2.57	0.52
1:C:246:HIS:H	1:C:246:HIS:HD2	1.57	0.52
1:C:220:TRP:HB3	1:C:257:THR:HB	1.90	0.52
1:A:347:TYR:CA	1:A:356:VAL:HG22	2.39	0.52
1:A:367:ILE:HG13	1:A:408:LEU:HG	1.91	0.52
1:C:37:THR:HG22	1:C:39:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD22	1:A:130:LEU:N	2.24	0.52
1:A:86:TRP:HD1	1:A:124:ASN:ND2	2.08	0.51
1:A:94:LYS:HE2	4:A:488:HOH:O	2.10	0.51
1:C:214:ASP:C	1:C:216:THR:N	2.59	0.51
1:A:381:PRO:O	1:A:387:GLY:HA2	2.10	0.51
1:B:265:TYR:CE2	1:B:267:TRP:HB2	2.45	0.51
1:A:90:LEU:HD21	1:A:142:LYS:HB3	1.91	0.51
1:A:379:TRP:CE3	1:A:389:ILE:CG2	2.94	0.51
1:A:68:TRP:CZ2	1:A:78:VAL:CG1	2.89	0.51
1:A:87:GLU:O	1:A:91:LEU:N	2.37	0.51
1:B:357:ILE:H	1:B:357:ILE:HD12	1.75	0.51
1:A:81:LEU:CD2	1:A:119:ILE:HB	2.39	0.51
1:C:198:LEU:HD22	1:C:250:PHE:O	2.09	0.51
1:A:347:TYR:CB	1:A:356:VAL:HG22	2.41	0.51
1:A:389:ILE:HG23	1:A:389:ILE:O	2.09	0.51
1:C:156:ARG:HG2	1:C:162:ILE:HG22	1.91	0.51
1:A:93:ILE:HD11	1:A:379:TRP:CG	2.45	0.51
1:A:380:ASN:O	1:A:388:GLY:CA	2.59	0.51
1:A:73:THR:HB	1:A:75:ASN:ND2	2.25	0.51
1:C:131:ASP:OD1	1:C:134:GLN:HG3	2.11	0.51
1:C:35:THR:HG21	1:C:39:ILE:H	1.75	0.51
1:A:130:LEU:HB3	1:A:134:GLN:HE21	1.76	0.51
1:A:77:VAL:CG1	1:A:78:VAL:N	2.74	0.50
1:B:320:PRO:HD3	1:B:361:LYS:HZ3	1.76	0.50
1:C:110:VAL:HA	1:C:133:LEU:HD13	1.92	0.50
1:C:85:ASN:HD21	1:C:87:GLU:HB2	1.75	0.50
1:A:94:LYS:HG3	1:A:95:SER:N	2.25	0.50
1:C:208:PRO:HB2	1:C:212:TYR:CE2	2.46	0.50
1:C:219:THR:HG22	1:C:227:THR:O	2.12	0.50
1:A:201:GLU:O	1:A:203:HIS:HD2	1.95	0.50
1:C:201:GLU:O	1:C:203:HIS:CD2	2.65	0.50
1:A:152:LEU:HD11	1:A:187:PHE:HB3	1.93	0.50
1:A:405:LEU:CB	4:A:515:HOH:O	2.56	0.50
1:C:377:TRP:CZ2	2:C:2739:CTT:H3B	2.47	0.50
1:C:316:PRO:HG3	1:C:357:ILE:HG21	1.94	0.50
1:A:156:ARG:CB	1:A:158:GLY:O	2.59	0.49
1:A:84:ARG:CZ	1:A:394:TRP:O	2.59	0.49
1:B:200:ASN:ND2	1:B:201:GLU:HG3	2.27	0.49
1:C:220:TRP:NE1	1:C:230:ASN:HB3	2.26	0.49
1:B:181:ILE:O	1:B:185:LYS:HG3	2.12	0.49
1:A:389:ILE:O	1:A:390:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TYR:CE2	1:A:356:VAL:HG13	2.48	0.49
1:A:73:THR:OG1	1:A:75:ASN:ND2	2.45	0.49
1:A:253:GLY:O	1:A:274:GLY:HA2	2.13	0.49
1:A:397:ILE:HD13	1:A:397:ILE:O	2.13	0.49
1:A:87:GLU:O	1:A:91:LEU:HG	2.13	0.49
1:B:177:ILE:O	1:B:181:ILE:HG13	2.12	0.49
1:C:219:THR:HG23	1:C:228:ASP:HA	1.94	0.49
1:C:85:ASN:ND2	1:C:88:ASP:H	2.05	0.49
1:B:68:TRP:HZ2	4:B:549:HOH:O	1.95	0.49
1:A:68:TRP:HB3	1:A:103:LEU:CD2	2.42	0.49
1:A:212:TYR:CD2	1:A:259:PRO:HD3	2.46	0.49
1:A:389:ILE:O	1:A:390:LEU:CB	2.57	0.49
1:A:393:ASP:O	1:A:395:THR:N	2.42	0.49
1:B:68:TRP:CZ3	1:B:79:HIS:O	2.66	0.49
1:A:266:LYS:HE2	1:A:267:TRP:HE1	1.77	0.49
1:A:135:ILE:HD12	1:A:139:ILE:HG13	1.95	0.49
1:B:203:HIS:HE1	4:B:512:HOH:O	1.96	0.49
1:B:259:PRO:O	1:B:263:SER:OG	2.26	0.49
1:B:380:ASN:HB3	1:B:382:ASP:OD1	2.13	0.49
1:A:90:LEU:HD22	1:A:142:LYS:CG	2.43	0.48
1:B:201:GLU:O	1:B:203:HIS:HD2	1.95	0.48
1:C:71:PHE:CE1	1:C:77:VAL:HA	2.48	0.48
1:A:94:LYS:HB2	1:A:94:LYS:NZ	2.28	0.48
1:A:380:ASN:C	1:A:388:GLY:CA	2.82	0.48
1:B:200:ASN:CG	1:B:201:GLU:HG3	2.34	0.48
1:C:270:ASN:OD1	1:C:307:PRO:HG3	2.14	0.48
1:A:85:ASN:CA	1:A:124:ASN:HD21	2.24	0.48
1:A:130:LEU:CD2	1:A:130:LEU:N	2.77	0.48
1:A:155:HIS:HA	1:A:200:ASN:CB	2.44	0.48
1:A:234:GLU:OE1	1:A:286:ASN:HB3	2.14	0.48
1:A:331:LYS:HB2	1:A:338:VAL:CG2	2.44	0.48
1:A:77:VAL:HG12	1:A:78:VAL:N	2.28	0.48
1:A:73:THR:HB	1:A:75:ASN:HD21	1.77	0.47
1:C:187:PHE:HA	1:C:190:TYR:HD2	1.79	0.47
1:A:391:GLN:HB2	1:A:396:THR:HG23	1.95	0.47
1:C:332:LEU:HD21	1:C:369:ASN:HB3	1.97	0.47
1:A:376:TYR:CD2	1:A:389:ILE:HG12	2.50	0.47
1:B:86:TRP:CH2	1:B:142:LYS:HG3	2.50	0.47
1:C:166:TRP:NE1	1:C:173:GLU:OE1	2.43	0.47
1:A:385:ASP:OD1	2:A:2739:CTT:H5D	2.14	0.47
1:A:347:TYR:HA	1:A:356:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PHE:CZ	1:A:382:ASP:OD1	2.67	0.47
1:A:73:THR:CB	1:A:75:ASN:ND2	2.77	0.47
1:A:68:TRP:CE3	1:A:380:ASN:ND2	2.81	0.47
1:A:69:PHE:O	1:A:78:VAL:HA	2.13	0.47
1:A:132:SER:O	1:A:136:MET:HB2	2.15	0.47
1:A:155:HIS:HA	1:A:200:ASN:HB3	1.97	0.47
1:B:107:THR:O	1:B:111:LYS:HG2	2.15	0.47
1:A:76:HIS:HB2	1:A:116:PRO:HA	1.96	0.47
1:A:366:MET:CB	1:A:408:LEU:HD11	2.43	0.47
1:B:75:ASN:ND2	4:B:516:HOH:O	2.47	0.47
1:C:381:PRO:HD2	1:C:394:TRP:CH2	2.49	0.47
1:A:161:HIS:N	1:A:161:HIS:CD2	2.82	0.47
1:A:346:LYS:HE3	1:A:386:THR:HA	1.95	0.47
1:A:69:PHE:CD2	1:A:377:TRP:CZ2	3.03	0.47
1:A:49:TYR:OH	1:C:54:THR:HG21	2.15	0.47
1:B:222:MET:SD	1:B:259:PRO:HD3	2.55	0.47
1:C:406:LYS:O	1:C:410:ASP:N	2.47	0.47
1:A:267:TRP:CE3	1:A:308:TYR:HD2	2.32	0.47
1:C:340:ILE:HD12	1:C:366:MET:HE3	1.96	0.47
1:A:347:TYR:CG	1:A:356:VAL:HA	2.50	0.46
1:A:402:TYR:OH	1:A:406:LYS:CE	2.64	0.46
1:B:73:THR:OG1	1:B:79:HIS:HE1	1.98	0.46
1:A:128:ARG:C	1:A:130:LEU:HD22	2.36	0.46
1:A:42:GLU:OE2	1:A:44:ARG:NE	2.43	0.46
1:A:302:ASP:HB3	1:A:385:ASP:O	2.15	0.46
1:A:349:HIS:O	1:A:350:GLY:C	2.54	0.46
1:B:316:PRO:HG3	1:B:357:ILE:CG2	2.45	0.46
1:B:79:HIS:CD2	1:B:382:ASP:OD2	2.67	0.46
1:C:295:SER:HA	1:C:339:VAL:O	2.15	0.46
1:C:380:ASN:O	1:C:388:GLY:HA3	2.15	0.46
1:C:315:PHE:HD1	1:C:319:LEU:HD11	1.79	0.46
1:C:69:PHE:HB2	1:C:72:GLU:OE2	2.16	0.46
1:A:69:PHE:HZ	1:A:382:ASP:OD1	1.99	0.46
1:B:409:MET:O	1:B:410:ASP:OD1	2.33	0.46
1:A:135:ILE:O	1:A:139:ILE:HG12	2.15	0.46
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.28	0.46
1:A:91:LEU:N	4:A:473:HOH:O	2.47	0.46
1:B:380:ASN:N	1:B:380:ASN:ND2	2.60	0.46
1:A:316:PRO:O	1:A:319:LEU:HB2	2.15	0.46
1:A:72:GLU:HG3	1:A:155:HIS:HD2	1.81	0.46
1:A:80:GLY:HA3	1:A:394:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:PHE:HA	1:C:316:PRO:HA	1.70	0.46
1:A:71:PHE:CD2	1:A:103:LEU:HD22	2.51	0.46
1:A:37:THR:HG22	1:A:39:ILE:N	2.27	0.46
1:C:246:HIS:N	1:C:246:HIS:CD2	2.84	0.46
1:A:131:ASP:OD2	1:A:134:GLN:NE2	2.49	0.46
1:A:135:ILE:HD12	1:A:139:ILE:CG1	2.46	0.45
1:C:163:GLU:CD	1:C:163:GLU:H	2.19	0.45
1:C:68:TRP:HD1	1:C:380:ASN:HD21	1.63	0.45
1:A:331:LYS:HB2	1:A:338:VAL:HG23	1.99	0.45
1:A:69:PHE:C	1:A:69:PHE:CD1	2.89	0.45
1:B:287:LEU:HD12	1:B:292:LEU:HD13	1.98	0.45
1:C:281:LYS:CB	1:C:281:LYS:NZ	2.79	0.45
1:C:209:PRO:HA	1:C:212:TYR:HD2	1.82	0.45
1:A:123:LYS:O	1:A:125:PRO:HD3	2.16	0.45
1:A:93:ILE:CD1	1:A:379:TRP:CE3	2.99	0.45
1:B:299:TYR:HE2	4:B:529:HOH:O	1.99	0.45
1:B:75:ASN:ND2	1:B:79:HIS:CE1	2.84	0.45
1:A:291:LYS:HE2	1:A:291:LYS:HA	1.97	0.45
1:C:74:PRO:HD3	1:C:159:CYS:O	2.17	0.45
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.81	0.45
1:C:304:TYR:CD2	3:C:459:CBI:H5'	2.51	0.45
1:C:35:THR:HG21	1:C:39:ILE:N	2.32	0.45
1:B:85:ASN:ND2	1:B:87:GLU:HB3	2.31	0.45
1:C:219:THR:HG21	1:C:227:THR:OG1	2.16	0.45
1:C:331:LYS:HB2	1:C:338:VAL:HG23	1.99	0.45
1:A:100:ALA:HA	1:A:148:ILE:HG23	1.98	0.45
1:A:68:TRP:HH2	1:A:89:MET:HE3	1.82	0.45
1:B:57:GLU:HG3	1:B:58:GLU:N	2.32	0.45
1:A:143:ALA:O	1:A:148:ILE:HB	2.17	0.45
1:A:94:LYS:HE3	1:A:98:PHE:O	2.17	0.45
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.52	0.44
1:C:319:LEU:N	1:C:319:LEU:HD12	2.30	0.44
1:A:77:VAL:HG22	1:A:135:ILE:HG12	1.99	0.44
1:C:162:ILE:O	1:C:162:ILE:HG13	2.16	0.44
1:C:292:LEU:HG	1:C:293:VAL:N	2.31	0.44
1:B:357:ILE:HD12	1:B:357:ILE:N	2.32	0.44
1:A:86:TRP:N	1:A:124:ASN:HD21	2.14	0.44
1:A:134:GLN:HG2	1:A:134:GLN:H	1.55	0.44
1:A:306:GLN:O	1:A:309:PHE:HB2	2.16	0.44
1:A:383:SER:HB3	1:A:387:GLY:N	2.32	0.44
1:A:64:PHE:CG	1:A:409:MET:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LYS:HB2	1:B:406:LYS:HZ2	1.81	0.44
1:A:36:PRO:HG2	1:A:37:THR:H	1.83	0.44
1:B:380:ASN:H	1:B:380:ASN:ND2	1.97	0.44
1:A:65:GLY:CA	1:A:100:ALA:O	2.66	0.44
1:C:330:VAL:HG12	1:C:336:TYR:CB	2.45	0.44
1:A:144:GLY:CA	4:A:501:HOH:O	2.56	0.44
1:A:152:LEU:HD11	1:A:187:PHE:CB	2.48	0.44
1:C:219:THR:HG22	1:C:227:THR:OG1	2.17	0.44
1:A:153:ASP:OD1	1:A:153:ASP:C	2.55	0.44
1:A:267:TRP:CZ2	1:A:313:LYS:HG2	2.52	0.44
1:C:316:PRO:HA	1:C:319:LEU:CD1	2.48	0.44
1:A:295:SER:HA	1:A:339:VAL:O	2.18	0.44
1:A:134:GLN:O	1:A:135:ILE:C	2.54	0.43
1:A:397:ILE:HG12	1:A:398:TRP:N	2.32	0.43
1:A:86:TRP:H	1:A:124:ASN:ND2	2.14	0.43
1:C:316:PRO:CA	1:C:319:LEU:HD13	2.48	0.43
1:A:272:TRP:CZ3	1:A:304:TYR:HB3	2.52	0.43
1:A:381:PRO:HD2	1:A:394:TRP:CZ3	2.53	0.43
1:B:238:LYS:NZ	4:B:514:HOH:O	2.48	0.43
1:C:188:GLY:O	1:C:246:HIS:HE1	2.00	0.43
1:A:121:TYR:N	1:A:121:TYR:CD1	2.86	0.43
1:A:123:LYS:C	1:A:125:PRO:HD3	2.38	0.43
1:C:262:ASP:HA	1:C:278:MET:HE3	2.00	0.43
1:C:35:THR:CG2	1:C:39:ILE:O	2.60	0.43
1:A:68:TRP:CD2	1:A:78:VAL:HG21	2.54	0.43
1:B:406:LYS:CB	1:B:406:LYS:NZ	2.82	0.43
1:A:36:PRO:HG2	1:A:37:THR:N	2.34	0.43
1:A:383:SER:C	1:A:385:ASP:N	2.70	0.43
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.57	0.43
1:C:37:THR:HG21	1:C:191:TRP:CB	2.49	0.43
1:A:346:LYS:HG2	4:A:492:HOH:O	2.18	0.43
1:A:354:ARG:HG3	1:A:357:ILE:HD12	2.01	0.43
1:C:286:ASN:ND2	4:C:464:HOH:O	2.42	0.43
1:A:164:PRO:HG3	1:A:205:VAL:CG1	2.49	0.43
1:A:289:ARG:NH2	1:A:336:TYR:CZ	2.87	0.43
1:C:35:THR:HA	1:C:36:PRO:HD3	1.83	0.43
1:A:119:ILE:HD11	1:A:121:TYR:OH	2.19	0.43
1:A:379:TRP:CG	1:A:379:TRP:O	2.72	0.43
1:A:141:LYS:HA	1:A:141:LYS:HD3	1.83	0.43
1:A:398:TRP:HB3	1:A:401:LYS:CB	2.49	0.43
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ARG:CG	1:C:289:ARG:O	2.67	0.43
1:A:80:GLY:CA	1:A:394:TRP:CE2	3.02	0.42
1:C:302:ASP:HB3	1:C:385:ASP:O	2.18	0.42
1:C:65:GLY:HA2	1:C:100:ALA:O	2.18	0.42
1:B:188:GLY:O	1:B:246:HIS:HE1	2.02	0.42
1:C:265:TYR:CD1	1:C:266:LYS:N	2.87	0.42
1:A:381:PRO:CG	1:A:394:TRP:CE2	3.02	0.42
1:A:90:LEU:CD2	1:A:142:LYS:HB3	2.49	0.42
1:B:142:LYS:O	1:B:146:LEU:HD13	2.19	0.42
1:C:49:TYR:HE1	1:C:60:PRO:HG3	1.82	0.42
1:A:386:THR:C	1:A:387:GLY:O	2.57	0.42
1:A:38:GLY:O	1:A:53:VAL:HG22	2.20	0.42
1:A:381:PRO:CA	1:A:388:GLY:N	2.72	0.42
1:A:379:TRP:CZ3	1:A:389:ILE:CG2	3.03	0.42
1:A:68:TRP:HE3	1:A:380:ASN:ND2	2.14	0.42
1:A:93:ILE:HG22	1:A:94:LYS:N	2.34	0.42
1:C:201:GLU:CD	2:C:2739:CTT:O1B	2.58	0.42
1:C:34:GLN:HA	1:C:34:GLN:OE1	2.19	0.42
1:A:110:VAL:O	1:A:133:LEU:HD22	2.19	0.42
1:A:316:PRO:HG3	1:A:357:ILE:CG2	2.50	0.42
1:A:68:TRP:HB3	1:A:103:LEU:HD23	2.01	0.42
1:B:86:TRP:CZ3	1:B:142:LYS:HG3	2.55	0.42
1:B:187:PHE:HA	1:B:190:TYR:HD2	1.84	0.42
1:B:87:GLU:OE2	1:B:142:LYS:NZ	2.47	0.42
1:C:292:LEU:HD21	1:C:294:TYR:CE2	2.54	0.42
1:B:161:HIS:HE1	4:B:508:HOH:O	2.02	0.42
1:B:35:THR:HA	1:B:36:PRO:HD3	1.76	0.42
1:C:42:GLU:OE2	1:C:51:ILE:CD1	2.68	0.42
1:C:172:SER:O	1:C:175:ASP:HB2	2.20	0.42
1:C:319:LEU:H	1:C:319:LEU:CD1	2.33	0.42
1:C:319:LEU:HD21	1:C:358:TRP:HD1	1.85	0.42
1:A:346:LYS:CE	1:A:386:THR:C	2.88	0.42
1:A:72:GLU:OE2	2:A:2739:CTT:O6E	2.25	0.42
1:A:73:THR:HB	1:A:74:PRO:CD	2.45	0.42
1:A:94:LYS:HD3	1:A:94:LYS:C	2.40	0.42
1:C:198:LEU:CD2	1:C:250:PHE:O	2.68	0.42
1:C:242:LYS:HE3	1:C:242:LYS:HB2	1.86	0.42
1:C:283:TYR:N	1:C:284:PRO:CD	2.83	0.42
1:C:345:GLY:HA3	1:C:355:ASP:OD2	2.20	0.42
1:A:131:ASP:O	1:A:133:LEU:CA	2.67	0.41
1:A:222:MET:SD	1:A:259:PRO:HD2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:HA	1:A:401:LYS:CG	2.49	0.41
1:A:35:THR:HB	1:A:246:HIS:HB3	2.01	0.41
1:B:246:HIS:N	1:B:246:HIS:CD2	2.86	0.41
1:C:271:ALA:HB1	1:C:276:ASN:HB2	2.01	0.41
1:C:316:PRO:HG3	1:C:357:ILE:HG22	2.02	0.41
1:A:74:PRO:O	1:A:76:HIS:ND1	2.39	0.41
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.83	0.41
1:A:81:LEU:HB3	1:A:119:ILE:HG22	2.02	0.41
1:A:199:LYS:HB3	1:A:229:TRP:CH2	2.55	0.41
1:A:376:TYR:OH	1:A:401:LYS:HD3	2.21	0.41
1:C:279:ALA:O	1:C:283:TYR:HB2	2.21	0.41
1:A:135:ILE:O	1:A:135:ILE:HD12	2.21	0.41
1:A:106:CYS:HA	1:A:156:ARG:O	2.20	0.41
1:A:267:TRP:CE2	1:A:308:TYR:HB3	2.55	0.41
1:A:68:TRP:CD1	1:A:78:VAL:HG21	2.55	0.41
1:A:93:ILE:O	1:A:96:LEU:HB2	2.20	0.41
1:B:42:GLU:OE2	1:B:58:GLU:OE2	2.38	0.41
1:A:379:TRP:CZ3	1:A:389:ILE:HG22	2.55	0.41
1:B:77:VAL:O	1:B:78:VAL:C	2.59	0.41
1:C:257:THR:OG1	1:C:258:ASN:N	2.52	0.41
1:C:323:TRP:CH2	1:C:362:LEU:HA	2.55	0.41
1:C:368:GLU:C	1:C:370:LYS:H	2.24	0.41
1:C:304:TYR:CE2	3:C:459:CBI:H5'	2.56	0.41
1:A:100:ALA:HA	1:A:149:PHE:O	2.21	0.41
1:A:344:GLY:HA2	1:A:376:TYR:CE1	2.56	0.41
1:A:383:SER:OG	1:A:385:ASP:OD2	2.37	0.41
1:A:72:GLU:N	1:A:72:GLU:OE1	2.44	0.41
1:A:398:TRP:HB3	1:A:401:LYS:HB3	2.01	0.41
1:B:206:THR:O	1:B:211:ALA:HB2	2.21	0.41
1:C:180:TRP:CE3	1:C:183:VAL:HG21	2.56	0.41
1:C:205:VAL:CG2	1:C:216:THR:O	2.63	0.41
1:A:130:LEU:CB	1:A:134:GLN:HE21	2.34	0.41
1:C:184:ALA:HA	1:C:247:TRP:CH2	2.55	0.41
1:A:316:PRO:HG3	1:A:357:ILE:HG21	2.04	0.40
1:A:133:LEU:HA	1:A:133:LEU:HD12	1.70	0.40
1:A:343:PHE:O	1:A:377:TRP:N	2.40	0.40
1:A:347:TYR:CG	1:A:356:VAL:HG13	2.56	0.40
1:A:72:GLU:OE2	2:A:2739:CTT:C6E	2.70	0.40
1:C:198:LEU:HD21	1:C:249:ILE:HG22	1.98	0.40
1:A:315:PHE:HA	1:A:316:PRO:HA	1.85	0.40
1:C:173:GLU:O	1:C:177:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASP:HA	1:C:250:PHE:HB2	2.03	0.40
1:C:46:ASP:OD1	1:C:46:ASP:C	2.60	0.40
1:B:299:TYR:CD1	1:B:303:VAL:HG21	2.56	0.40
1:C:331:LYS:HB2	1:C:338:VAL:CG2	2.51	0.40
1:C:131:ASP:OD1	1:C:134:GLN:CG	2.70	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:554:HOH:O	4:C:500:HOH:O[4_545]	2.03	0.17
4:B:553:HOH:O	4:C:553:HOH:O[4_545]	2.10	0.10
1:A:95:SER:OG	1:A:354:ARG:NH1[4_556]	2.16	0.04

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	375/458 (82%)	338 (90%)	31 (8%)	6 (2%)	11	5
1	B	375/458 (82%)	361 (96%)	14 (4%)	0	100	100
1	C	375/458 (82%)	354 (94%)	20 (5%)	1 (0%)	44	40
All	All	1125/1374 (82%)	1053 (94%)	65 (6%)	7 (1%)	28	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	384	GLY
1	A	390	LEU
1	A	112	PRO
1	C	215	GLY

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Mol	Chain	Res	Type
1	A	327	PHE
1	A	350	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/395 (82%)	285 (88%)	38 (12%)	6	3
1	B	323/395 (82%)	311 (96%)	12 (4%)	39	36
1	C	323/395 (82%)	306 (95%)	17 (5%)	26	21
All	All	969/1185 (82%)	902 (93%)	67 (7%)	18	12

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	68	TRP
1	A	69	PHE
1	A	75	ASN
1	A	78	VAL
1	A	79	HIS
1	A	87	GLU
1	A	88	ASP
1	A	92	GLN
1	A	94	LYS
1	A	112	PRO
1	A	126	ASP
1	A	130	LEU
1	A	134	GLN
1	A	135	ILE
1	A	141	LYS
1	A	153	ASP
1	A	154	TYR
1	A	180	TRP
1	A	190	TYR

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Mol	Chain	Res	Type
1	A	281	LYS
1	A	290	ASN
1	A	297	HIS
1	A	313	LYS
1	A	319	LEU
1	A	326	HIS
1	A	343	PHE
1	A	346	LYS
1	A	347	TYR
1	A	354	ARG
1	A	389	ILE
1	A	390	LEU
1	A	392	ASP
1	A	393	ASP
1	A	396	THR
1	A	397	ILE
1	A	399	GLU
1	A	408	LEU
1	B	57	GLU
1	B	68	TRP
1	B	115	GLN
1	B	142	LYS
1	B	153	ASP
1	B	154	TYR
1	B	241	LEU
1	B	246	HIS
1	B	297	HIS
1	B	380	ASN
1	B	399	GLU
1	B	406	LYS
1	C	58	GLU
1	C	138	LYS
1	C	154	TYR
1	C	160	THR
1	C	214	ASP
1	C	246	HIS
1	C	260	LYS
1	C	270	ASN
1	C	282	ASP
1	C	287	LEU
1	C	289	ARG
1	C	297	HIS

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Mol	Chain	Res	Type
1	C	317	ASP
1	C	334	LEU
1	C	380	ASN
1	C	407	ARG
1	C	410	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	75	ASN
1	A	85	ASN
1	A	124	ASN
1	A	134	GLN
1	A	161	HIS
1	A	203	HIS
1	A	246	HIS
1	A	290	ASN
1	A	297	HIS
1	A	325	HIS
1	A	359	GLN
1	B	62	HIS
1	B	75	ASN
1	B	79	HIS
1	B	85	ASN
1	B	115	GLN
1	B	161	HIS
1	B	178	ASN
1	B	203	HIS
1	B	246	HIS
1	B	270	ASN
1	B	297	HIS
1	B	325	HIS
1	B	326	HIS
1	B	349	HIS
1	B	359	GLN
1	B	380	ASN
1	B	391	GLN
1	C	62	HIS
1	C	75	ASN
1	C	79	HIS
1	C	85	ASN

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Mol	Chain	Res	Type
1	C	203	HIS
1	C	246	HIS
1	C	255	GLN
1	C	270	ASN
1	C	297	HIS
1	C	325	HIS
1	C	349	HIS
1	C	359	GLN
1	C	380	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CTT	A	2739	-	48,48,48	0.84	1 (2%)	71,71,71	1.38	11 (15%)
2	CTT	B	2739	-	48,48,48	0.92	1 (2%)	71,71,71	1.30	4 (5%)
2	CTT	C	2739	-	48,48,48	0.98	2 (4%)	71,71,71	1.50	9 (12%)
3	CBI	C	459	-	24,24,24	0.45	0	35,35,35	0.96	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTT	A	2739	-	-	0/20/100/100	0/4/4/4
2	CTT	B	2739	-	-	0/20/100/100	0/4/4/4
2	CTT	C	2739	-	-	0/20/100/100	0/4/4/4
3	CBI	C	459	-	-	0/8/48/48	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2739	CTT	O5B-C5B	2.09	1.49	1.44
2	C	2739	CTT	O5D-C1D	2.14	1.47	1.41
2	C	2739	CTT	O5B-C1B	2.26	1.47	1.43
2	B	2739	CTT	O5B-C1B	2.27	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2739	CTT	C1B-C2B-C3B	-5.69	100.37	110.65
2	B	2739	CTT	C1B-C2B-C3B	-4.55	102.44	110.65
2	C	2739	CTT	C1B-O5B-C5B	-4.43	105.40	113.39
2	B	2739	CTT	C1B-O5B-C5B	-3.88	106.39	113.39
2	A	2739	CTT	C1B-O5B-C5B	-3.75	106.62	113.39
2	A	2739	CTT	C1D-O4C-C4C	-3.52	109.43	118.00
2	A	2739	CTT	C1B-C2B-C3B	-3.50	104.32	110.65
2	A	2739	CTT	C1C-O4B-C4B	-3.24	110.09	118.00
2	A	2739	CTT	C1D-C2D-C3D	-2.83	104.72	109.98
2	C	2739	CTT	O4B-C4B-C5B	-2.58	103.00	109.34
3	C	459	CBI	C1'-O5'-C5'	-2.48	108.91	113.39
2	C	2739	CTT	C1D-O4C-C4C	-2.44	112.05	118.00
2	A	2739	CTT	C1D-O5D-C5D	-2.34	109.31	113.72
2	A	2739	CTT	C1E-O5E-C5E	-2.26	109.46	113.72
2	B	2739	CTT	C1D-O4C-C4C	-2.23	112.56	118.00
2	C	2739	CTT	C6E-C5E-C4E	-2.21	107.82	113.00
2	A	2739	CTT	O2B-C2B-C3B	-2.19	105.59	110.36
2	A	2739	CTT	C6B-C5B-C4B	-2.18	107.28	113.24
2	C	2739	CTT	O2B-C2B-C3B	-2.16	105.66	110.36
2	A	2739	CTT	C6C-C5C-C4C	-2.10	107.50	113.24
3	C	459	CBI	C3'-C4'-C5'	-2.08	106.46	110.88
2	A	2739	CTT	C1E-C2E-C3E	-2.07	106.14	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2739	CTT	C1D-C2D-C3D	-2.03	106.20	109.98
2	B	2739	CTT	O4B-C4B-C3B	2.20	112.48	107.19
2	C	2739	CTT	O5B-C1B-C2B	2.26	113.78	110.04
2	C	2739	CTT	O4B-C4B-C3B	3.30	115.14	107.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2739	CTT	3	0
2	C	2739	CTT	2	0
3	C	459	CBI	2	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	377/458 (82%)	0.54	35 (9%) 9 9	26, 52, 84, 113	2 (0%)
1	B	377/458 (82%)	-0.11	10 (2%) 55 54	20, 33, 55, 85	3 (0%)
1	C	377/458 (82%)	0.62	57 (15%) 3 3	29, 56, 81, 101	2 (0%)
All	All	1131/1374 (82%)	0.35	102 (9%) 10 10	20, 46, 79, 113	7 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	6.7
1	C	269	TYR	5.6
1	A	122	SER	5.6
1	C	151	LEU	5.4
1	C	342	ALA	4.8
1	C	216	THR	4.6
1	C	53	VAL	4.6
1	C	340	ILE	4.6
1	A	349	HIS	4.5
1	C	217	GLY	4.4
1	C	205	VAL	4.3
1	C	375	PHE	4.2
1	A	128	ARG	4.1
1	C	265	TYR	3.9
1	C	102	ARG	3.8
1	C	264	SER	3.8
1	A	129	GLY	3.8
1	B	170	ASP	3.8
1	C	315	PHE	3.8
1	C	101	ILE	3.7
1	C	152	LEU	3.7
1	C	66	VAL	3.6
1	C	267	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	295	SER	3.5
1	C	251	VAL	3.4
1	C	250	PHE	3.4
1	C	263	SER	3.3
1	A	394	TRP	3.3
1	C	208	PRO	3.3
1	A	379	TRP	3.3
1	C	341	GLY	3.2
1	A	377	TRP	3.1
1	C	332	LEU	3.1
1	C	311	PRO	3.1
1	C	339	VAL	3.1
1	A	118	GLY	3.1
1	C	103	LEU	3.1
1	A	53	VAL	3.0
1	C	206	THR	3.0
1	C	54	THR	2.9
1	C	334	LEU	2.9
1	A	342	ALA	2.9
1	A	340	ILE	2.9
1	A	344	GLY	2.9
1	A	135	ILE	2.8
1	C	104	PRO	2.8
1	C	214	ASP	2.8
1	C	150	VAL	2.7
1	B	104	PRO	2.7
1	A	375	PHE	2.7
1	C	212	TYR	2.7
1	A	142	LYS	2.7
1	B	151	LEU	2.7
1	A	267	TRP	2.6
1	C	196	ALA	2.6
1	A	121	TYR	2.6
1	C	211	ALA	2.6
1	C	336	TYR	2.5
1	A	88	ASP	2.4
1	A	80	GLY	2.4
1	C	45	GLY	2.4
1	A	136	MET	2.4
1	A	35	THR	2.4
1	A	82	TRP	2.4
1	C	58	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	380	ASN	2.4
1	A	95	SER	2.4
1	B	171	PHE	2.3
1	C	343	PHE	2.3
1	C	243	VAL	2.3
1	C	262	ASP	2.3
1	C	194	ILE	2.3
1	C	63	LEU	2.3
1	B	68	TRP	2.3
1	C	260	LYS	2.3
1	C	170	ASP	2.2
1	A	38	GLY	2.2
1	C	207	SER	2.2
1	A	119	ILE	2.2
1	C	374	PHE	2.2
1	A	296	PRO	2.2
1	B	295	SER	2.2
1	A	130	LEU	2.2
1	C	195	GLY	2.2
1	B	169	GLU	2.1
1	A	138	LYS	2.1
1	A	346	LYS	2.1
1	B	375	PHE	2.1
1	C	283	TYR	2.1
1	B	250	PHE	2.1
1	C	153	ASP	2.1
1	C	65	GLY	2.1
1	A	89	MET	2.1
1	C	143	ALA	2.0
1	C	171	PHE	2.0
1	C	309	PHE	2.0
1	B	102	ARG	2.0
1	A	159	CYS	2.0
1	C	197	ASP	2.0
1	A	83	LYS	2.0
1	A	390	LEU	2.0
1	C	198	LEU	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 [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	CTT	B	2739	45/45	0.87	0.15	1.22	23,35,47,66	0
2	CTT	C	2739	45/45	0.86	0.15	0.46	40,57,68,76	0
2	CTT	A	2739	45/45	0.89	0.14	-0.04	38,56,70,72	0
3	CBI	C	459	23/23	0.86	0.12	-0.59	58,68,75,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.