Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:21 PM BST

PDB ID	:	3EE6
Title	:	Crystal Structure Analysis of Tripeptidyl peptidase -I
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Deposited on	:	2008-09-04
Resolution	:	2.35 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
https://www.wwpdb.org/validation/2017/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:

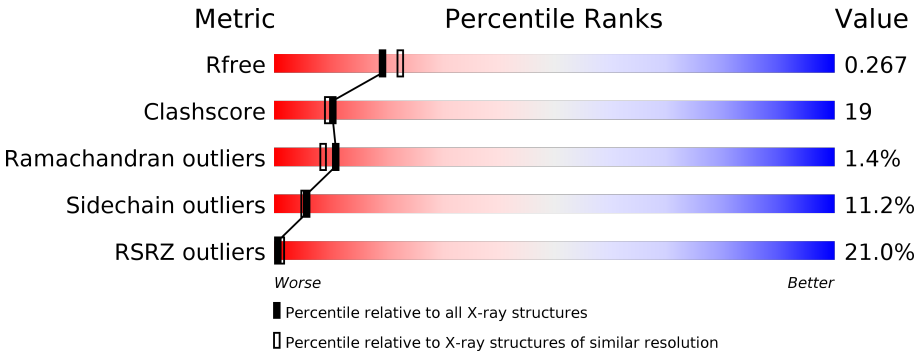
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 respectively. 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 <=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	571	17% 65% 23% 5% 7%
1	B	571	22% 62% 24% 6% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	575	-	-	-	X
2	NAG	B	575	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8361 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.

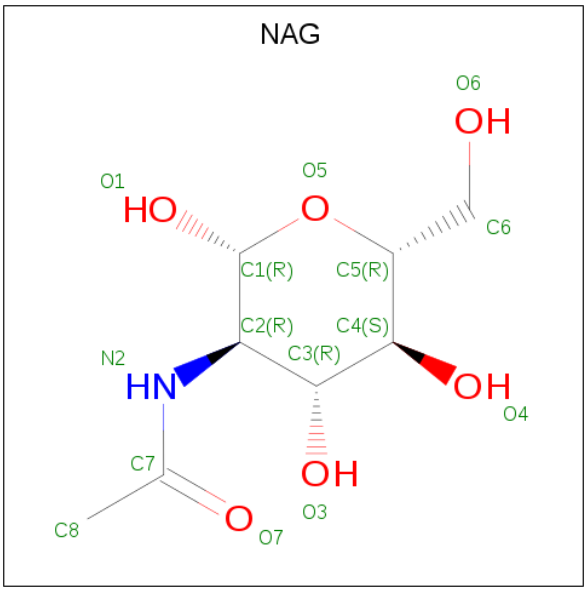
- Molecule 1 is a protein called Tripeptidyl-peptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4082	2588	714	769	11			
1	B	529	Total	C	N	O	S	0	0	0
			4080	2587	714	768	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	ARG	-	expression tag	UNP O14773
A	565	SER	-	expression tag	UNP O14773
A	566	HIS	-	expression tag	UNP O14773
A	567	HIS	-	expression tag	UNP O14773
A	568	HIS	-	expression tag	UNP O14773
A	569	HIS	-	expression tag	UNP O14773
A	570	HIS	-	expression tag	UNP O14773
A	571	HIS	-	expression tag	UNP O14773
B	564	ARG	-	expression tag	UNP O14773
B	565	SER	-	expression tag	UNP O14773
B	566	HIS	-	expression tag	UNP O14773
B	567	HIS	-	expression tag	UNP O14773
B	568	HIS	-	expression tag	UNP O14773
B	569	HIS	-	expression tag	UNP O14773
B	570	HIS	-	expression tag	UNP O14773
B	571	HIS	-	expression tag	UNP O14773

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 13 8 1 4	0	0
2	A	1	Total C N O 13 8 1 4	0	0
2	A	1	Total C N O 13 8 1 4	0	0
2	A	1	Total C N O 13 8 1 4	0	0
2	B	1	Total C N O 13 8 1 4	0	0
2	B	1	Total C N O 13 8 1 4	0	0
2	B	1	Total C N O 13 8 1 4	0	0
2	B	1	Total C N O 13 8 1 4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Zn 4 4	0	0
3	A	4	Total Zn 4 4	0	0

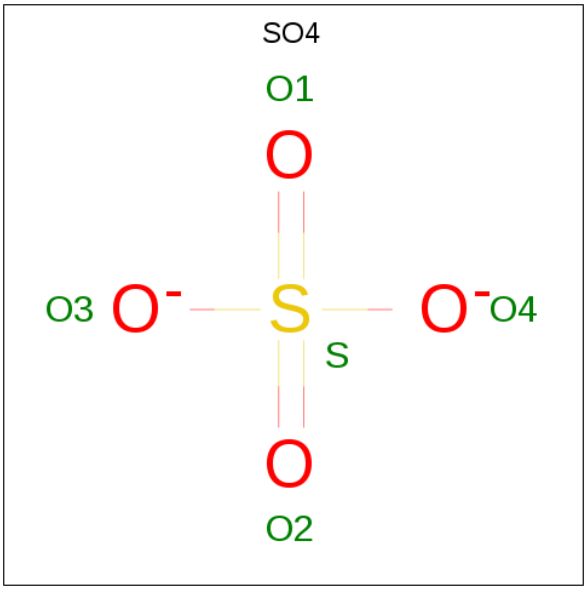
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	36	Total O 36 36	0	0

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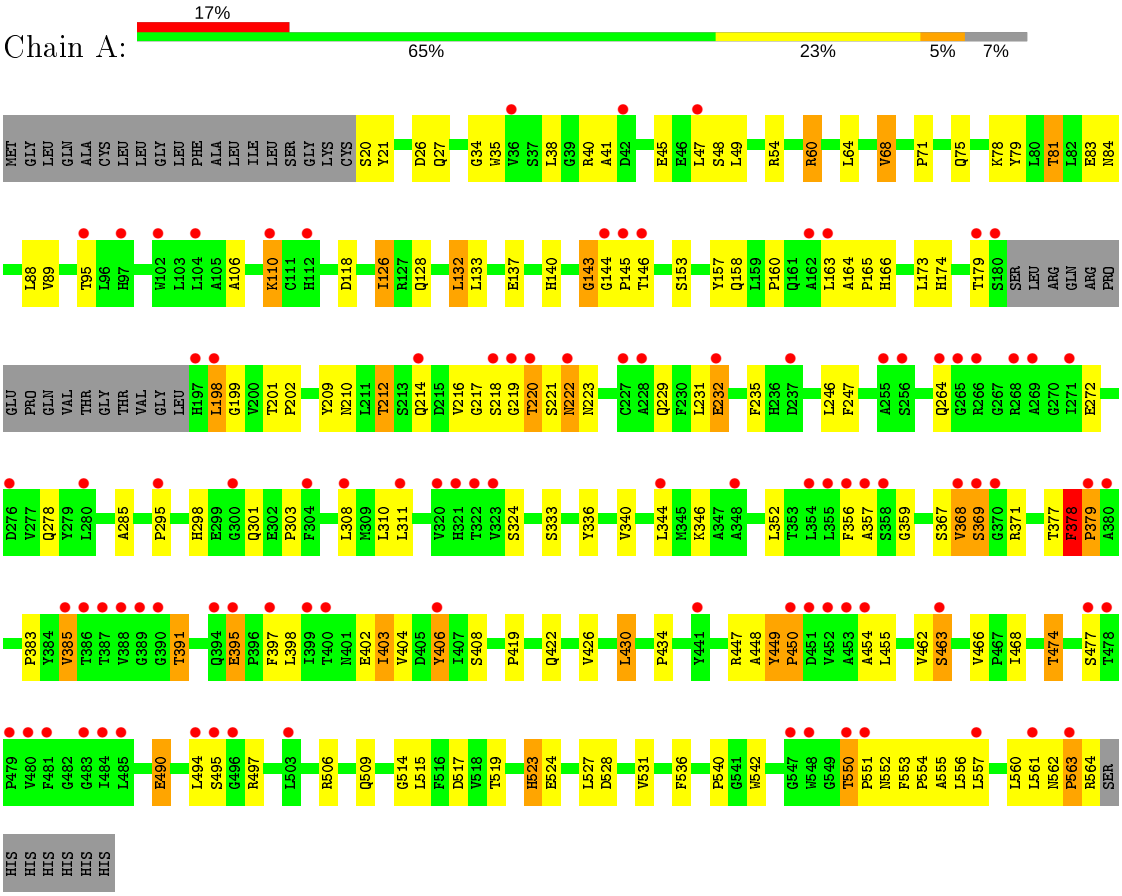
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	37	Total O 37 37	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

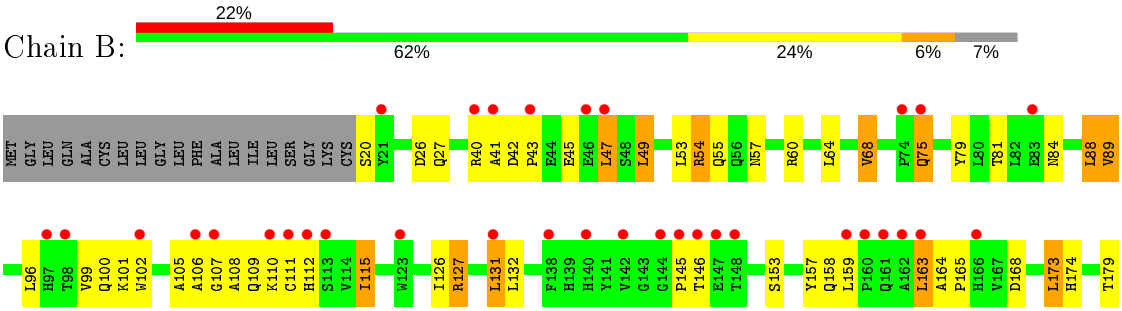
- Molecule 1: Tripeptidyl-peptidase 1

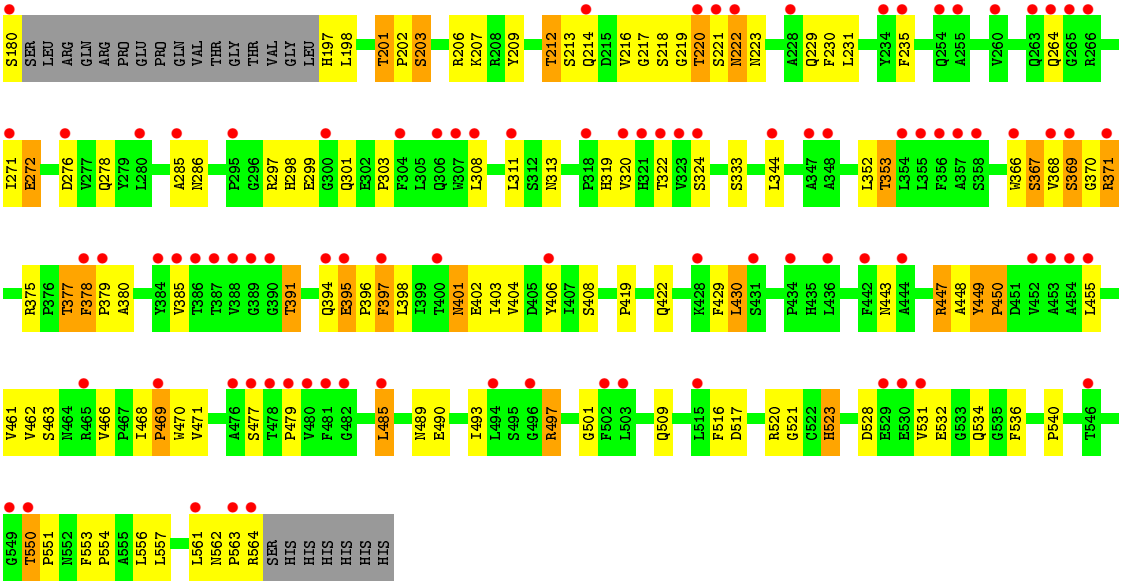
Chain A:



- Molecule 1: Tripeptidyl-peptidase 1

Chain B:




S180 SER LEU ARG GLN ARG PRO GLU PRO GLN VAL THR GLY THR VAL GLY LEU H197 L198 T201 P202 S203 R206 K207 R208 Y209 T212 S213 Q214 D215 V216 G217 S218 G219 T220 S221 N222 N223 A228 Q229 F230 L231 Y234 F235 Q254 A255 V260 Q263 Q264 G265 R266
I271 E272 D276 V277 Q278 Y279 L280 A285 N286 P295 G296 R297 H298 E299 G300 Q301 E302 P303 F304 L305 Q306 W307 L308 L311 S312 N313 P318 H319 V320 H321 T322 V323 S324 S333 L344 A347 A348 L352 T353 L354 L355 F356 A357 S358 W366 S367 V368 S369 G370 R371
R375 P376 T377 F378 P379 A380 Y384 V385 T386 T387 V388 G389 G390 T391 Q394 E395 P396 F397 L398 I399 T400 N401 E402 I403 V404 D405 Y406 I407 S408 P419 Q422 K428 F429 L430 S431 P434 H435 L436 F442 N443 A444 R447 A448 Y449 P450 D451 V452 A453 A454 L455
V461 V462 S463 N464 R465 V466 P467 I468 P469 W470 V471 A476 S477 T478 P479 V480 F481 G482 L485 N489 E490 I493 L494 S495 G496 R497 G501 F502 L503 Q509 L515 F516 D517 R520 G521 C522 H523 D528 E529 E530 V531 E532 G533 Q534 G535 F536 P540 T546
G549 T550 P551 N552 F553 P554 A555 L556 L557 L561 N562 P563 R564 SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	113.45Å 128.93Å 100.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.21 – 2.35 39.21 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.21-2.35) 99.6 (39.21-2.35)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.218 , 0.262 0.225 , 0.267	Depositor DCC
R_{free} test set	3150 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 70.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8361	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, ZN, CA, NAG, CL

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	0.52	0/4204	0.75	2/5741 (0.0%)
1	B	0.48	0/4202	0.71	1/5739 (0.0%)
All	All	0.50	0/8406	0.73	3/11480 (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	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	378	PHE	C-N-CD	-9.12	100.54	120.60
1	B	378	PHE	C-N-CD	-7.35	104.42	120.60
1	A	450	PRO	N-CA-C	-5.52	97.75	112.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	PHE	Peptide
1	A	449	TYR	Peptide
1	B	378	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	449	TYR	Mainchain,Peptide

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	4082	0	3900	138	0
1	B	4080	0	3901	164	0
2	A	52	0	44	0	0
2	B	52	0	44	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	36	0	0	0	0
7	B	37	0	0	2	0
All	All	8361	0	7889	301	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 19.

All (301) 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:562:ASN:HB3	1:A:563:PRO:CD	1.57	1.33
1:A:562:ASN:CB	1:A:563:PRO:HD3	1.69	1.20
1:A:95:THR:HG22	1:A:166:HIS:ND1	1.56	1.20
1:A:20:SER:OG	1:A:158:GLN:NE2	1.78	1.17
1:B:368:VAL:HG12	1:B:369:SER:H	1.04	1.16
1:A:146:THR:CB	1:A:232:GLU:HG2	1.82	1.09
1:B:563:PRO:O	4:B:580:CL:CL	2.09	1.08
1:B:212:THR:HG22	1:B:214:GLN:H	1.19	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ARG:NH1	1:A:561:LEU:O	1.92	1.03
1:B:101:LYS:HG3	1:B:102:TRP:N	1.71	1.02
1:B:368:VAL:HG12	1:B:369:SER:N	1.71	1.01
1:B:102:TRP:CZ3	1:B:163:LEU:HD11	1.99	0.97
1:B:371:ARG:HH11	1:B:371:ARG:CB	1.77	0.97
1:A:391:THR:HG22	1:A:455:LEU:HA	1.48	0.96
1:B:368:VAL:CG1	1:B:369:SER:H	1.77	0.96
1:A:357:ALA:HB1	1:A:474:THR:HG23	1.48	0.95
1:B:96:LEU:O	1:B:100:GLN:HG3	1.69	0.92
1:A:146:THR:CB	1:A:232:GLU:CG	2.49	0.90
1:B:102:TRP:CE3	1:B:163:LEU:HD11	2.07	0.89
1:A:34:GLY:O	1:A:143:GLY:O	1.90	0.89
1:A:463:SER:O	1:A:466:VAL:HG12	1.72	0.88
1:A:391:THR:HG21	1:A:402:GLU:OE1	1.72	0.87
1:A:562:ASN:HB3	1:A:563:PRO:HD3	0.87	0.87
1:A:368:VAL:HG12	1:A:369:SER:N	1.88	0.86
1:B:422:GLN:HE22	1:B:448:ALA:H	1.23	0.85
1:B:371:ARG:HH11	1:B:371:ARG:HB3	1.41	0.84
1:A:41:ALA:HB1	1:A:126:ILE:HD13	1.60	0.83
1:B:391:THR:HG22	1:B:455:LEU:HA	1.58	0.83
1:A:81:THR:HG22	1:A:84:ASN:H	1.45	0.82
1:B:209:TYR:CE2	1:B:550:THR:HG23	2.15	0.81
1:B:404:VAL:HG22	1:B:521:GLY:HA3	1.60	0.81
1:B:497:ARG:NH1	1:B:561:LEU:HD22	1.96	0.81
1:B:368:VAL:O	1:B:369:SER:C	2.18	0.81
1:B:102:TRP:CE3	1:B:163:LEU:CD1	2.63	0.81
1:B:531:VAL:HG12	1:B:531:VAL:O	1.79	0.81
1:B:209:TYR:HE2	1:B:550:THR:CG2	1.93	0.81
1:B:216:VAL:CG1	1:B:217:GLY:N	2.45	0.80
1:B:209:TYR:CE2	1:B:550:THR:CG2	2.66	0.79
1:A:41:ALA:HB1	1:A:126:ILE:CD1	2.13	0.79
1:B:105:ALA:O	1:B:106:ALA:HB3	1.83	0.78
1:B:391:THR:HG21	1:B:402:GLU:OE1	1.81	0.78
1:B:497:ARG:HH12	1:B:561:LEU:HD22	1.49	0.78
1:B:230:PHE:O	1:B:297:ARG:NH1	2.17	0.77
1:B:81:THR:HG23	1:B:84:ASN:H	1.48	0.77
1:A:216:VAL:CG1	1:A:217:GLY:N	2.48	0.77
1:A:357:ALA:HB1	1:A:474:THR:CG2	2.14	0.77
1:B:127:ARG:O	1:B:131:LEU:HD23	1.86	0.76
1:A:229:GLN:HE22	1:A:231:LEU:HB2	1.48	0.76
1:B:353:THR:HB	1:B:501:GLY:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:VAL:HG12	1:A:369:SER:H	1.48	0.76
1:A:41:ALA:CB	1:A:126:ILE:HD13	2.15	0.76
1:B:216:VAL:HG22	1:B:285:ALA:HB3	1.68	0.76
1:A:402:GLU:OE2	1:A:550:THR:HG21	1.85	0.76
1:B:216:VAL:HG12	1:B:217:GLY:N	1.99	0.75
1:B:563:PRO:O	1:B:564:ARG:HB2	1.86	0.75
1:A:517:ASP:OD2	1:A:540:PRO:O	2.04	0.75
1:B:497:ARG:NH2	1:B:561:LEU:O	2.21	0.74
1:B:550:THR:HG23	1:B:551:PRO:HD2	1.69	0.73
1:B:371:ARG:NH1	1:B:371:ARG:CB	2.51	0.73
1:B:497:ARG:HH21	1:B:563:PRO:HA	1.53	0.73
1:A:212:THR:HG23	1:A:214:GLN:H	1.54	0.72
1:B:229:GLN:HE22	1:B:231:LEU:HB2	1.54	0.72
1:A:422:GLN:HE22	1:A:448:ALA:H	1.34	0.72
1:B:101:LYS:HG3	1:B:102:TRP:H	1.54	0.72
1:A:562:ASN:CB	1:A:563:PRO:CD	2.38	0.72
1:B:109:GLN:O	1:B:111:CYS:SG	2.48	0.72
1:B:371:ARG:HH11	1:B:371:ARG:HB2	1.55	0.71
1:B:212:THR:CG2	1:B:214:GLN:H	1.99	0.70
1:B:371:ARG:NH1	1:B:371:ARG:HB2	2.05	0.70
1:A:157:TYR:CD2	1:A:173:LEU:HD23	2.25	0.70
1:A:391:THR:HG22	1:A:455:LEU:CA	2.20	0.70
1:A:527:LEU:HD22	1:B:406:TYR:OH	1.91	0.70
1:A:216:VAL:HG12	1:A:217:GLY:N	2.05	0.70
1:A:198:LEU:HD23	1:A:199:GLY:H	1.57	0.70
1:A:81:THR:HG23	1:A:83:GLU:H	1.55	0.70
1:B:497:ARG:NH1	1:B:561:LEU:CD2	2.56	0.69
1:A:562:ASN:HB3	1:A:563:PRO:HD2	1.72	0.69
1:B:212:THR:HG22	1:B:214:GLN:N	2.01	0.68
1:A:223:ASN:HD22	1:A:490:GLU:HG3	1.59	0.68
1:B:102:TRP:CH2	1:B:163:LEU:HD11	2.29	0.68
1:A:209:TYR:CE2	1:A:550:THR:HG23	2.29	0.68
1:B:402:GLU:OE2	1:B:550:THR:HG21	1.93	0.68
1:A:563:PRO:O	1:A:564:ARG:HG3	1.93	0.68
1:B:201:THR:HG23	1:B:202:PRO:HD2	1.76	0.68
1:B:115:ILE:HD13	1:B:313:ASN:OD1	1.93	0.67
1:A:132:LEU:HD13	1:A:133:LEU:HD21	1.75	0.67
1:B:107:GLY:O	1:B:108:ALA:C	2.32	0.67
1:B:100:GLN:O	1:B:101:LYS:CG	2.43	0.67
1:A:35:TRP:CZ3	1:A:143:GLY:HA2	2.31	0.66
1:A:81:THR:H	1:A:84:ASN:HD22	1.40	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:HG22	1:B:203:SER:H	1.60	0.66
1:B:517:ASP:OD2	1:B:540:PRO:O	2.14	0.66
1:B:497:ARG:NH2	1:B:563:PRO:HA	2.10	0.66
1:B:209:TYR:HE2	1:B:550:THR:HG21	1.58	0.66
1:A:157:TYR:CD2	1:A:173:LEU:CD2	2.80	0.65
1:B:216:VAL:CG1	1:B:217:GLY:H	2.11	0.64
1:B:217:GLY:O	1:B:286:ASN:HB3	1.96	0.64
1:B:463:SER:O	1:B:466:VAL:HG12	1.97	0.64
1:A:359:GLY:H	1:A:474:THR:HG21	1.62	0.64
1:B:299:GLU:OE1	1:B:299:GLU:N	2.30	0.64
1:A:426:VAL:HG12	1:A:430:LEU:HD22	1.79	0.63
1:A:35:TRP:CE3	1:A:143:GLY:HA2	2.33	0.63
1:B:53:LEU:HD22	1:B:99:VAL:HG21	1.80	0.63
1:B:377:THR:HG22	1:B:380:ALA:HB3	1.81	0.62
1:B:449:TYR:HB2	1:B:450:PRO:HA	1.81	0.62
1:B:531:VAL:HG13	1:B:534:GLN:O	2.00	0.61
1:A:223:ASN:HD22	1:A:490:GLU:CG	2.13	0.61
1:B:497:ARG:HH21	1:B:563:PRO:CA	2.14	0.61
1:B:497:ARG:NH2	1:B:562:ASN:O	2.35	0.60
1:A:132:LEU:HD13	1:A:133:LEU:CD2	2.31	0.60
1:B:531:VAL:CG1	1:B:531:VAL:O	2.47	0.60
1:B:100:GLN:O	1:B:102:TRP:N	2.28	0.59
1:B:367:SER:HA	1:B:371:ARG:O	2.03	0.59
1:B:368:VAL:CG1	1:B:369:SER:N	2.43	0.59
1:A:563:PRO:O	4:A:580:CL:CL	2.57	0.59
1:B:57:ASN:HB2	1:B:88:LEU:HD22	1.84	0.58
1:A:132:LEU:C	1:A:133:LEU:HD23	2.24	0.58
1:A:563:PRO:O	1:A:564:ARG:CG	2.51	0.58
1:B:223:ASN:HD22	1:B:490:GLU:HG3	1.69	0.58
1:A:144:GLY:O	1:A:146:THR:N	2.37	0.58
1:B:216:VAL:HG13	1:B:217:GLY:H	1.67	0.58
1:A:216:VAL:CG1	1:A:217:GLY:H	2.15	0.57
1:A:298:HIS:CD2	1:A:298:HIS:H	2.21	0.57
1:B:197:HIS:HA	1:B:396:PRO:O	2.04	0.57
1:A:422:GLN:NE2	1:A:448:ALA:H	2.00	0.57
1:B:229:GLN:HE21	1:B:272:GLU:HG2	1.69	0.57
1:B:466:VAL:HG13	1:B:468:ILE:HD11	1.87	0.57
1:A:466:VAL:HG13	1:A:468:ILE:HD11	1.87	0.56
1:A:216:VAL:HG13	1:A:217:GLY:H	1.70	0.56
1:A:368:VAL:CG1	1:A:369:SER:H	2.12	0.56
1:B:489:ASN:O	1:B:493:ILE:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD21	1:A:340:VAL:HG13	1.86	0.56
1:B:218:SER:O	1:B:220:THR:N	2.39	0.56
1:B:101:LYS:CG	1:B:102:TRP:N	2.56	0.56
1:B:102:TRP:CD2	1:B:163:LEU:HD11	2.40	0.56
1:B:391:THR:HG22	1:B:455:LEU:CA	2.33	0.56
1:A:144:GLY:C	1:A:146:THR:N	2.57	0.56
1:B:320:VAL:HG22	1:B:353:THR:HG23	1.88	0.55
1:A:45:GLU:HB3	1:A:126:ILE:HD12	1.88	0.55
1:A:110:LYS:CE	1:A:110:LYS:HA	2.37	0.55
1:B:201:THR:HG22	1:B:203:SER:N	2.22	0.54
1:B:20:SER:OG	1:B:158:GLN:NE2	2.41	0.54
1:B:212:THR:CG2	1:B:213:SER:N	2.70	0.54
1:A:216:VAL:HG22	1:A:285:ALA:HB3	1.90	0.54
1:A:110:LYS:HE3	1:A:110:LYS:HA	1.89	0.54
1:A:95:THR:CG2	1:A:166:HIS:ND1	2.50	0.54
1:B:229:GLN:NE2	1:B:272:GLU:HG2	2.22	0.54
1:B:102:TRP:CD2	1:B:163:LEU:CD1	2.90	0.53
1:B:404:VAL:CG2	1:B:521:GLY:HA3	2.37	0.53
1:B:550:THR:HG23	1:B:551:PRO:CD	2.38	0.53
1:A:550:THR:HG23	1:A:551:PRO:HD2	1.90	0.53
1:B:41:ALA:HB3	1:B:126:ILE:HD13	1.90	0.53
1:A:145:PRO:HD2	1:A:179:THR:HG23	1.91	0.52
1:B:216:VAL:HG13	1:B:286:ASN:H	1.75	0.52
1:B:216:VAL:HG22	1:B:285:ALA:CB	2.36	0.52
1:B:75:GLN:HA	1:B:75:GLN:HE21	1.74	0.52
1:B:100:GLN:O	1:B:101:LYS:HG2	2.09	0.52
1:A:160:PRO:HG2	1:A:163:LEU:HD23	1.92	0.52
1:A:81:THR:HG23	1:A:83:GLU:N	2.24	0.52
1:A:40:ARG:CZ	1:A:137:GLU:HG3	2.40	0.52
1:A:201:THR:CG2	1:A:202:PRO:HD2	2.40	0.52
1:A:367:SER:HA	1:A:371:ARG:O	2.09	0.51
1:B:153:SER:O	1:B:174:HIS:HD2	1.92	0.51
1:A:20:SER:OG	1:A:158:GLN:CD	2.46	0.51
1:A:209:TYR:CE2	1:A:550:THR:CG2	2.93	0.51
1:A:146:THR:CB	1:A:232:GLU:OE2	2.59	0.51
1:A:383:PRO:HB3	1:A:419:PRO:HG3	1.93	0.51
1:A:81:THR:HG22	1:A:84:ASN:N	2.21	0.51
1:A:556:LEU:HD22	1:A:560:LEU:HD12	1.92	0.50
1:A:494:LEU:O	1:A:495:SER:CB	2.60	0.50
1:A:218:SER:O	1:A:220:THR:N	2.44	0.49
1:B:102:TRP:CZ3	1:B:163:LEU:CD1	2.82	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:TYR:O	1:A:340:VAL:HG23	2.12	0.49
1:A:81:THR:H	1:A:84:ASN:ND2	2.08	0.49
1:A:359:GLY:N	1:A:474:THR:HG21	2.26	0.49
1:A:71:PRO:HG2	1:A:509:GLN:NE2	2.28	0.49
1:A:295:PRO:O	1:A:303:PRO:HA	2.13	0.49
1:B:27:GLN:HB2	1:B:333:SER:HB3	1.95	0.49
1:B:397:PHE:C	1:B:398:LEU:HD22	2.33	0.49
1:A:402:GLU:O	1:A:403:ILE:HD12	2.12	0.49
1:B:153:SER:O	1:B:174:HIS:CD2	2.66	0.49
1:B:298:HIS:HB3	1:B:299:GLU:OE1	2.13	0.48
1:A:201:THR:HG23	1:A:202:PRO:HD2	1.95	0.48
1:A:278:GLN:HE22	1:A:462:VAL:H	1.59	0.48
1:A:209:TYR:HE2	1:A:550:THR:CG2	2.27	0.48
1:A:27:GLN:HB2	1:A:333:SER:HB3	1.96	0.48
1:A:514:GLY:HA2	1:A:555:ALA:HB1	1.96	0.48
1:A:201:THR:HG22	1:A:202:PRO:N	2.29	0.48
1:A:146:THR:CB	1:A:232:GLU:CB	2.91	0.48
1:B:408:SER:O	1:B:523:HIS:HD2	1.97	0.48
1:A:391:THR:HG23	1:A:455:LEU:HD23	1.96	0.48
1:B:319:HIS:CD2	7:B:617:HOH:O	2.66	0.48
1:B:81:THR:HG22	1:B:84:ASN:ND2	2.29	0.48
1:A:391:THR:CG2	1:A:455:LEU:HD23	2.44	0.47
1:B:398:LEU:N	1:B:398:LEU:HD22	2.28	0.47
1:B:516:PHE:N	1:B:550:THR:O	2.46	0.47
1:A:528:ASP:C	1:A:528:ASP:OD1	2.52	0.47
1:A:81:THR:CG2	1:A:84:ASN:H	2.23	0.47
1:B:100:GLN:C	1:B:102:TRP:H	2.17	0.47
1:B:54:ARG:NH1	1:B:168:ASP:OD1	2.48	0.47
1:A:356:PHE:CE2	1:A:385:VAL:HG21	2.50	0.47
1:B:47:LEU:HD22	1:B:49:LEU:HD13	1.96	0.47
1:B:447:ARG:NH1	1:B:448:ALA:O	2.44	0.47
1:B:497:ARG:NH2	1:B:563:PRO:CA	2.76	0.47
1:B:100:GLN:C	1:B:102:TRP:N	2.67	0.47
1:A:519:THR:CG2	1:A:519:THR:O	2.63	0.47
1:B:212:THR:HG23	1:B:213:SER:N	2.30	0.47
1:B:366:TRP:HB2	1:B:375:ARG:HB2	1.97	0.47
1:A:41:ALA:CB	1:A:126:ILE:CD1	2.86	0.47
1:A:221:SER:OG	1:A:222:ASN:N	2.48	0.46
1:A:378:PHE:CD1	1:A:379:PRO:HA	2.51	0.46
1:B:101:LYS:CG	1:B:102:TRP:H	2.27	0.46
1:A:201:THR:HG23	1:A:247:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:CG1	1:B:286:ASN:HB2	2.45	0.46
1:B:297:ARG:C	1:B:299:GLU:H	2.17	0.46
1:A:157:TYR:CE2	1:A:173:LEU:HD22	2.50	0.46
1:B:553:PHE:HB3	1:B:554:PRO:HD3	1.97	0.46
1:B:561:LEU:C	1:B:562:ASN:O	2.51	0.46
1:B:206:ARG:NH2	1:B:285:ALA:HB2	2.30	0.46
1:B:297:ARG:C	1:B:299:GLU:N	2.68	0.46
1:A:406:TYR:CZ	1:A:524:GLU:HB3	2.51	0.46
1:A:519:THR:HG22	1:A:519:THR:O	2.14	0.46
1:B:109:GLN:O	1:B:110:LYS:C	2.55	0.45
1:B:201:THR:HG23	1:B:202:PRO:CD	2.44	0.45
1:B:485:LEU:HA	1:B:485:LEU:HD12	1.85	0.45
1:A:368:VAL:CG1	1:A:369:SER:N	2.57	0.45
1:B:105:ALA:O	1:B:106:ALA:CB	2.50	0.45
1:A:398:LEU:N	1:A:398:LEU:HD22	2.31	0.45
1:B:301:GLN:O	1:B:303:PRO:HD3	2.16	0.45
1:B:271:ILE:HD12	1:B:471:VAL:CG2	2.47	0.45
1:A:68:VAL:HG13	1:A:79:TYR:CE1	2.52	0.45
1:B:562:ASN:O	1:B:563:PRO:C	2.54	0.45
1:A:145:PRO:CD	1:A:179:THR:HG23	2.47	0.45
1:A:357:ALA:CB	1:A:474:THR:HG23	2.33	0.45
1:A:556:LEU:HD22	1:A:560:LEU:CD1	2.47	0.45
1:B:102:TRP:CE2	1:B:132:LEU:HD21	2.52	0.45
1:B:377:THR:HB	7:B:629:HOH:O	2.15	0.45
1:A:553:PHE:HB3	1:A:554:PRO:HD3	1.99	0.45
1:A:408:SER:O	1:A:523:HIS:HD2	2.00	0.44
1:B:41:ALA:CB	1:B:126:ILE:HD13	2.47	0.44
1:A:153:SER:O	1:A:174:HIS:HD2	2.00	0.44
1:A:514:GLY:HA2	1:A:555:ALA:CB	2.47	0.44
1:A:41:ALA:HB3	1:A:126:ILE:HD13	1.96	0.44
1:A:523:HIS:HE1	1:A:536:PHE:H	1.64	0.44
1:A:449:TYR:CD1	1:A:449:TYR:C	2.90	0.44
1:A:454:ALA:HB3	1:A:477:SER:HB2	1.99	0.44
1:B:395:GLU:CD	1:B:398:LEU:HB2	2.38	0.44
1:B:419:PRO:HD2	1:B:422:GLN:NE2	2.33	0.44
1:A:118:ASP:OD2	1:A:346:LYS:NZ	2.50	0.44
1:A:60:ARG:HD3	1:A:60:ARG:HA	1.74	0.44
1:B:369:SER:HB2	1:B:370:GLY:H	1.66	0.44
1:B:278:GLN:HE22	1:B:462:VAL:H	1.65	0.44
1:B:157:TYR:CD2	1:B:173:LEU:HD22	2.53	0.43
1:B:164:ALA:N	1:B:165:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ASP:O	1:B:532:GLU:HA	2.18	0.43
1:B:404:VAL:HG21	1:B:521:GLY:C	2.38	0.43
1:B:563:PRO:O	1:B:564:ARG:CB	2.56	0.43
1:B:75:GLN:CA	1:B:75:GLN:HE21	2.31	0.43
1:A:26:ASP:N	1:A:26:ASP:OD2	2.50	0.43
1:B:20:SER:HB2	1:B:159:LEU:O	2.18	0.43
1:B:394:GLN:HE21	1:B:401:ASN:HB3	1.84	0.43
1:A:210:ASN:ND2	1:A:552:ASN:OD1	2.51	0.43
1:A:216:VAL:HG13	1:A:285:ALA:O	2.17	0.43
1:A:132:LEU:CD1	1:A:133:LEU:HD21	2.46	0.43
1:B:229:GLN:HG3	1:B:272:GLU:HG3	2.00	0.43
1:B:469:PRO:HB2	1:B:470:TRP:CD1	2.54	0.43
1:A:128:GLN:O	1:A:132:LEU:HB2	2.19	0.43
1:B:497:ARG:NH2	1:B:562:ASN:C	2.72	0.43
1:B:26:ASP:OD2	1:B:26:ASP:N	2.52	0.43
1:B:81:THR:HG22	1:B:84:ASN:CG	2.38	0.43
1:A:301:GLN:O	1:A:303:PRO:HD3	2.19	0.42
1:A:448:ALA:HB1	1:A:542:TRP:HH2	1.83	0.42
1:A:395:GLU:CD	1:A:398:LEU:HB2	2.40	0.42
1:B:68:VAL:HG13	1:B:79:TYR:CE1	2.55	0.42
1:B:429:PHE:HD2	1:B:430:LEU:HD13	1.84	0.42
1:A:21:TYR:O	1:A:158:GLN:CB	2.68	0.42
1:B:221:SER:OG	1:B:222:ASN:N	2.52	0.42
1:B:523:HIS:HE1	1:B:536:PHE:H	1.68	0.42
1:A:391:THR:HG22	1:A:455:LEU:N	2.34	0.41
1:B:42:ASP:O	1:B:43:PRO:C	2.58	0.41
1:B:561:LEU:O	1:B:562:ASN:C	2.55	0.41
1:A:298:HIS:N	1:A:298:HIS:CD2	2.85	0.41
1:B:198:LEU:HD11	1:B:397:PHE:O	2.21	0.41
1:A:515:LEU:HD23	1:A:551:PRO:HA	2.01	0.41
1:B:320:VAL:HG22	1:B:353:THR:CG2	2.50	0.41
1:B:45:GLU:O	1:B:126:ILE:HG23	2.19	0.41
1:B:403:ILE:HG13	1:B:520:ARG:HB3	2.03	0.41
1:A:164:ALA:N	1:A:165:PRO:CD	2.84	0.41
1:A:21:TYR:O	1:A:158:GLN:HB2	2.20	0.41
1:B:297:ARG:O	1:B:299:GLU:N	2.54	0.41
1:A:144:GLY:O	1:A:146:THR:C	2.59	0.41
1:A:41:ALA:HA	1:A:140:HIS:CE1	2.56	0.41
1:A:106:ALA:HB2	1:A:132:LEU:HD23	2.01	0.41
1:B:201:THR:CG2	1:B:202:PRO:N	2.84	0.41
1:B:408:SER:O	1:B:523:HIS:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLN:HB3	1:B:89:VAL:HG22	2.02	0.41
1:B:229:GLN:HE21	1:B:231:LEU:HG	1.86	0.41
1:A:463:SER:O	1:A:466:VAL:CG1	2.56	0.40
1:B:322:THR:HG21	1:B:479:PRO:HA	2.02	0.40
1:B:179:THR:O	1:B:180:SER:C	2.60	0.40
1:B:556:LEU:HA	1:B:556:LEU:HD23	1.94	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	525/571 (92%)	495 (94%)	21 (4%)	9 (2%)	9 7
1	B	525/571 (92%)	479 (91%)	40 (8%)	6 (1%)	14 13
All	All	1050/1142 (92%)	974 (93%)	61 (6%)	15 (1%)	11 9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLY
1	A	368	VAL
1	B	219	GLY
1	B	369	SER
1	A	406	TYR
1	A	450	PRO
1	A	563	PRO
1	B	379	PRO
1	A	369	SER
1	B	450	PRO
1	A	379	PRO
1	A	434	PRO

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Mol	Chain	Res	Type
1	B	145	PRO
1	A	143	GLY
1	B	469	PRO

5.3.2 Protein sidechains (i)

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	443/479 (92%)	396 (89%)	47 (11%)	6 6
1	B	443/479 (92%)	391 (88%)	52 (12%)	5 5
All	All	886/958 (92%)	787 (89%)	99 (11%)	6 5

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	47	LEU
1	A	48	SER
1	A	49	LEU
1	A	54	ARG
1	A	60	ARG
1	A	64	LEU
1	A	68	VAL
1	A	75	GLN
1	A	78	LYS
1	A	81	THR
1	A	88	LEU
1	A	89	VAL
1	A	110	LYS
1	A	126	ILE
1	A	132	LEU
1	A	198	LEU
1	A	212	THR
1	A	220	THR
1	A	222	ASN

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Mol	Chain	Res	Type
1	A	232	GLU
1	A	235	PHE
1	A	246	LEU
1	A	264	GLN
1	A	272	GLU
1	A	310	LEU
1	A	311	LEU
1	A	324	SER
1	A	344	LEU
1	A	352	LEU
1	A	377	THR
1	A	385	VAL
1	A	391	THR
1	A	395	GLU
1	A	397	PHE
1	A	403	ILE
1	A	404	VAL
1	A	430	LEU
1	A	447	ARG
1	A	463	SER
1	A	474	THR
1	A	490	GLU
1	A	506	ARG
1	A	523	HIS
1	A	531	VAL
1	A	550	THR
1	A	557	LEU
1	B	40	ARG
1	B	47	LEU
1	B	49	LEU
1	B	54	ARG
1	B	60	ARG
1	B	64	LEU
1	B	68	VAL
1	B	75	GLN
1	B	88	LEU
1	B	89	VAL
1	B	112	HIS
1	B	115	ILE
1	B	127	ARG
1	B	131	LEU
1	B	146	THR

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Mol	Chain	Res	Type
1	B	163	LEU
1	B	173	LEU
1	B	201	THR
1	B	203	SER
1	B	207	LYS
1	B	212	THR
1	B	220	THR
1	B	222	ASN
1	B	235	PHE
1	B	264	GLN
1	B	272	GLU
1	B	276	ASP
1	B	308	LEU
1	B	311	LEU
1	B	324	SER
1	B	344	LEU
1	B	352	LEU
1	B	353	THR
1	B	367	SER
1	B	371	ARG
1	B	377	THR
1	B	385	VAL
1	B	391	THR
1	B	395	GLU
1	B	397	PHE
1	B	401	ASN
1	B	430	LEU
1	B	443	ASN
1	B	447	ARG
1	B	461	VAL
1	B	477	SER
1	B	485	LEU
1	B	497	ARG
1	B	509	GLN
1	B	523	HIS
1	B	550	THR
1	B	557	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN

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Mol	Chain	Res	Type
1	A	75	GLN
1	A	84	ASN
1	A	158	GLN
1	A	161	GLN
1	A	174	HIS
1	A	223	ASN
1	A	225	GLN
1	A	229	GLN
1	A	278	GLN
1	A	298	HIS
1	A	321	HIS
1	A	394	GLN
1	A	422	GLN
1	A	504	ASN
1	A	509	GLN
1	A	523	HIS
1	B	56	GLN
1	B	57	ASN
1	B	75	GLN
1	B	100	GLN
1	B	158	GLN
1	B	174	HIS
1	B	223	ASN
1	B	225	GLN
1	B	229	GLN
1	B	254	GLN
1	B	264	GLN
1	B	278	GLN
1	B	394	GLN
1	B	422	GLN
1	B	504	ASN
1	B	509	GLN
1	B	523	HIS
1	B	552	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	572	1	13,13,15	0.96	0	14,17,21	1.63	4 (28%)
2	NAG	A	572	1	13,13,15	1.00	0	14,17,21	1.04	1 (7%)
6	SO4	A	582	-	4,4,4	0.15	0	6,6,6	0.17	0
2	NAG	A	575	1	13,13,15	0.75	0	14,17,21	0.99	0
2	NAG	A	574	1	13,13,15	0.89	0	14,17,21	1.41	2 (14%)
2	NAG	B	574	1	13,13,15	1.22	2 (15%)	14,17,21	1.77	2 (14%)
2	NAG	B	573	1	13,13,15	0.99	0	14,17,21	1.32	3 (21%)
2	NAG	A	573	1	13,13,15	1.59	2 (15%)	14,17,21	2.52	7 (50%)
2	NAG	B	575	1	13,13,15	0.96	0	14,17,21	1.26	2 (14%)
6	SO4	B	582	-	4,4,4	0.15	0	6,6,6	0.19	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	NAG	B	572	1	-	2/6/19/26	1/1/1/1
2	NAG	A	572	1	-	4/6/19/26	1/1/1/1
2	NAG	A	575	1	-	5/6/19/26	0/1/1/1
2	NAG	A	574	1	-	3/6/19/26	0/1/1/1
2	NAG	B	574	1	-	2/6/19/26	0/1/1/1
2	NAG	B	573	1	-	5/6/19/26	0/1/1/1
2	NAG	A	573	1	-	4/6/19/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	575	1	-	6/6/19/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	573	NAG	C3-C2	4.01	1.56	1.52
2	A	573	NAG	C4-C3	2.82	1.57	1.52
2	B	574	NAG	C4-C3	2.61	1.57	1.52
2	B	574	NAG	C3-C2	2.06	1.54	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	573	NAG	C4-C3-C2	4.96	118.42	110.84
2	A	573	NAG	C3-C4-C5	-4.63	103.25	111.22
2	B	574	NAG	C4-C3-C2	4.30	117.41	110.84
2	A	574	NAG	O5-C1-C2	-3.65	105.53	111.29
2	B	574	NAG	O5-C1-C2	-3.43	105.87	111.29
2	A	573	NAG	C2-N2-C7	3.43	127.79	122.90
2	B	572	NAG	O5-C1-C2	-3.02	106.52	111.29
2	B	572	NAG	C3-C4-C5	-2.81	106.38	111.22
2	A	573	NAG	O5-C5-C4	2.76	115.12	110.65
2	B	575	NAG	C4-C3-C2	2.74	115.03	110.84
2	A	573	NAG	O7-C7-C8	-2.39	117.62	122.06
2	B	572	NAG	O3-C3-C2	-2.32	105.13	109.96
2	B	572	NAG	C4-C3-C2	2.28	114.33	110.84
2	B	575	NAG	O5-C1-C2	-2.26	107.73	111.29
2	A	572	NAG	C4-C5-C6	2.24	116.53	112.60
2	A	574	NAG	C4-C3-C2	2.17	114.15	110.84
2	B	573	NAG	O5-C1-C2	-2.15	107.89	111.29
2	A	573	NAG	O5-C1-C2	-2.07	108.02	111.29
2	B	573	NAG	C4-C5-C6	2.06	116.22	112.60
2	A	573	NAG	O7-C7-N2	2.03	125.68	121.95
2	B	573	NAG	C3-C4-C5	-2.01	107.75	111.22

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	574	NAG	C4-C5-C6-O6
2	B	574	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	572	NAG	C1-C2-N2-C7
2	A	572	NAG	C4-C5-C6-O6
2	A	572	NAG	C8-C7-N2-C2
2	A	572	NAG	O7-C7-N2-C2
2	B	573	NAG	C4-C5-C6-O6
2	B	573	NAG	O5-C5-C6-O6
2	A	573	NAG	C4-C5-C6-O6
2	A	573	NAG	O5-C5-C6-O6
2	B	575	NAG	C3-C2-N2-C7
2	B	575	NAG	C4-C5-C6-O6
2	B	575	NAG	O5-C5-C6-O6
2	B	575	NAG	C8-C7-N2-C2
2	B	575	NAG	O7-C7-N2-C2
2	A	573	NAG	C8-C7-N2-C2
2	A	573	NAG	O7-C7-N2-C2
2	A	575	NAG	C8-C7-N2-C2
2	A	575	NAG	O7-C7-N2-C2
2	B	572	NAG	C8-C7-N2-C2
2	A	574	NAG	C8-C7-N2-C2
2	A	574	NAG	O7-C7-N2-C2
2	B	572	NAG	O7-C7-N2-C2
2	A	574	NAG	C1-C2-N2-C7
2	B	573	NAG	C8-C7-N2-C2
2	A	575	NAG	O5-C5-C6-O6
2	B	573	NAG	O7-C7-N2-C2
2	A	575	NAG	C4-C5-C6-O6
2	B	573	NAG	C3-C2-N2-C7
2	B	575	NAG	C1-C2-N2-C7
2	A	575	NAG	C1-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	572	NAG	C1-C2-C3-C4-C5-O5
2	A	572	NAG	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	529/571 (92%)	1.11	96 (18%) 1 2	49, 67, 79, 88	0
1	B	529/571 (92%)	1.23	126 (23%) 0 1	60, 67, 79, 91	0
All	All	1058/1142 (92%)	1.17	222 (20%) 1 1	49, 67, 79, 91	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	THR	14.5
1	A	220	THR	11.1
1	A	388	VAL	8.0
1	A	255	ALA	7.7
1	A	265	GLY	7.7
1	A	198	LEU	7.3
1	B	369	SER	6.9
1	B	531	VAL	6.7
1	B	397	PHE	6.7
1	A	496	GLY	6.6
1	B	355	LEU	6.5
1	A	145	PRO	6.4
1	B	145	PRO	6.3
1	A	264	GLN	6.3
1	A	355	LEU	6.1
1	B	123	TRP	5.9
1	B	368	VAL	5.6
1	B	480	VAL	5.5
1	B	563	PRO	5.4
1	A	399	ILE	5.3
1	B	564	ARG	5.2
1	A	354	LEU	5.2
1	A	368	VAL	5.2
1	A	452	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	395	GLU	5.1
1	A	163	LEU	5.1
1	B	400	THR	5.0
1	B	323	VAL	4.7
1	B	180	SER	4.7
1	B	308	LEU	4.6
1	B	356	PHE	4.6
1	A	387	THR	4.6
1	B	453	ALA	4.5
1	A	369	SER	4.4
1	B	477	SER	4.4
1	A	222	ASN	4.4
1	A	563	PRO	4.4
1	B	214	GLN	4.4
1	A	454	ALA	4.2
1	A	478	THR	4.1
1	A	323	VAL	4.1
1	A	280	LEU	4.1
1	A	551	PRO	4.1
1	B	388	VAL	4.0
1	A	477	SER	4.0
1	A	162	ALA	4.0
1	B	371	ARG	3.9
1	A	453	ALA	3.9
1	A	295	PRO	3.9
1	A	344	LEU	3.9
1	A	480	VAL	3.9
1	A	197	HIS	3.9
1	B	163	LEU	3.9
1	B	386	THR	3.8
1	B	479	PRO	3.8
1	A	481	PHE	3.8
1	B	160	PRO	3.8
1	A	397	PHE	3.8
1	A	180	SER	3.8
1	A	300	GLY	3.7
1	B	102	TRP	3.7
1	A	400	THR	3.7
1	B	454	ALA	3.7
1	B	387	THR	3.7
1	B	254	GLN	3.6
1	B	322	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	265	GLY	3.6
1	B	146	THR	3.6
1	B	21	TYR	3.6
1	A	219	GLY	3.5
1	A	451	ASP	3.5
1	B	112	HIS	3.5
1	A	389	GLY	3.5
1	B	260	VAL	3.5
1	B	234	TYR	3.5
1	A	385	VAL	3.5
1	A	386	THR	3.5
1	A	485	LEU	3.5
1	A	112	HIS	3.5
1	B	264	GLN	3.4
1	A	450	PRO	3.4
1	B	496	GLY	3.4
1	A	110	LYS	3.4
1	B	494	LEU	3.4
1	B	354	LEU	3.4
1	B	97	HIS	3.3
1	B	481	PHE	3.3
1	A	547	GLY	3.3
1	A	214	GLN	3.3
1	A	256	SER	3.3
1	B	222	ASN	3.3
1	B	147	GLU	3.3
1	B	311	LEU	3.2
1	A	356	PHE	3.2
1	A	494	LEU	3.2
1	B	142	VAL	3.1
1	B	221	SER	3.1
1	B	110	LYS	3.1
1	A	104	LEU	3.1
1	A	394	GLN	3.1
1	A	479	PRO	3.1
1	A	232	GLU	3.1
1	A	268	ARG	3.1
1	B	357	ALA	3.1
1	B	348	ALA	3.0
1	A	321	HIS	3.0
1	B	295	PRO	3.0
1	B	148	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	530	GLU	2.9
1	A	218	SER	2.9
1	B	300	GLY	2.9
1	B	307	TRP	2.9
1	B	46	GLU	2.9
1	B	366	TRP	2.9
1	A	483	GLY	2.9
1	B	389	GLY	2.9
1	A	146	THR	2.9
1	A	320	VAL	2.9
1	A	406	TYR	2.9
1	A	484	ILE	2.8
1	B	478	THR	2.8
1	B	107	GLY	2.8
1	A	503	LEU	2.8
1	B	406	TYR	2.8
1	B	138	PHE	2.8
1	B	321	HIS	2.8
1	A	269	ALA	2.8
1	B	561	LEU	2.8
1	A	97	HIS	2.8
1	B	75	GLN	2.7
1	B	379	PRO	2.7
1	B	159	LEU	2.7
1	B	347	ALA	2.7
1	B	131	LEU	2.7
1	A	390	GLY	2.7
1	B	74	PRO	2.7
1	A	308	LEU	2.7
1	B	358	SER	2.7
1	B	436	LEU	2.7
1	B	228	ALA	2.6
1	B	455	LEU	2.6
1	A	102	TRP	2.6
1	A	95	THR	2.6
1	B	550	THR	2.6
1	A	561	LEU	2.6
1	B	285	ALA	2.6
1	B	378	PHE	2.6
1	B	304	PHE	2.6
1	A	266	ARG	2.6
1	B	166	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	255	ALA	2.5
1	A	348	ALA	2.5
1	B	390	GLY	2.5
1	A	322	THR	2.5
1	A	370	GLY	2.5
1	B	113	SER	2.5
1	B	385	VAL	2.5
1	B	442	PHE	2.4
1	B	271	ILE	2.4
1	B	266	ARG	2.4
1	B	503	LEU	2.4
1	B	320	VAL	2.4
1	B	469	PRO	2.4
1	B	549	GLY	2.4
1	B	324	SER	2.4
1	B	111	CYS	2.4
1	B	144	GLY	2.4
1	A	550	THR	2.4
1	B	546	THR	2.4
1	A	304	PHE	2.4
1	B	476	ALA	2.3
1	B	98	THR	2.3
1	B	106	ALA	2.3
1	B	465	ARG	2.3
1	A	276	ASP	2.3
1	B	452	VAL	2.3
1	B	502	PHE	2.3
1	B	161	GLN	2.3
1	B	263	GLN	2.3
1	B	344	LEU	2.3
1	A	237	ASP	2.3
1	B	276	ASP	2.3
1	A	47	LEU	2.3
1	B	384	TYR	2.3
1	A	42	ASP	2.3
1	B	431	SER	2.3
1	B	434	PRO	2.2
1	A	357	ALA	2.2
1	B	482	GLY	2.2
1	B	43	PRO	2.2
1	B	306	GLN	2.2
1	B	529	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	40	ARG	2.2
1	A	395	GLU	2.2
1	B	140	HIS	2.2
1	A	358	SER	2.2
1	B	428	LYS	2.2
1	A	311	LEU	2.2
1	B	394	GLN	2.2
1	A	557	LEU	2.1
1	A	380	ALA	2.1
1	B	235	PHE	2.1
1	B	444	ALA	2.1
1	A	144	GLY	2.1
1	B	162	ALA	2.1
1	A	379	PRO	2.1
1	A	463	SER	2.1
1	B	47	LEU	2.1
1	B	515	LEU	2.1
1	A	227	CYS	2.1
1	B	83	GLU	2.1
1	A	495	SER	2.1
1	B	485	LEU	2.1
1	A	228	ALA	2.1
1	A	36	VAL	2.1
1	A	441	TYR	2.1
1	B	280	LEU	2.0
1	B	318	PRO	2.0
1	A	548	TRP	2.0
1	B	41	ALA	2.0
1	A	271	ILE	2.0
1	A	179	THR	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	NAG	A	575	13/15	0.22	0.42	87,88,90,91	0
2	NAG	B	575	13/15	0.53	0.44	88,90,93,93	0
2	NAG	A	573	13/15	0.74	0.21	68,72,79,80	0
3	ZN	B	579	1/1	0.74	0.29	116,116,116,116	0
2	NAG	A	572	13/15	0.77	0.21	82,85,89,90	0
2	NAG	B	574	13/15	0.78	0.22	81,83,85,85	0
3	ZN	B	576	1/1	0.80	0.09	87,87,87,87	1
3	ZN	A	579	1/1	0.81	0.11	114,114,114,114	0
6	SO4	B	582	5/5	0.84	0.30	104,104,105,105	0
6	SO4	A	582	5/5	0.84	0.40	112,112,112,112	0
2	NAG	B	573	13/15	0.85	0.19	69,74,79,80	0
2	NAG	A	574	13/15	0.85	0.16	80,81,84,85	0
4	CL	A	580	1/1	0.88	0.27	98,98,98,98	0
4	CL	B	580	1/1	0.88	0.20	112,112,112,112	0
2	NAG	B	572	13/15	0.90	0.09	72,73,77,78	0
5	CA	B	581	1/1	0.92	0.07	61,61,61,61	0
3	ZN	A	576	1/1	0.94	0.14	91,91,91,91	0
3	ZN	A	577	1/1	0.95	0.06	71,71,71,71	1
3	ZN	B	577	1/1	0.96	0.09	94,94,94,94	0
3	ZN	B	578	1/1	0.97	0.09	90,90,90,90	0
3	ZN	A	578	1/1	0.97	0.18	83,83,83,83	0
5	CA	A	581	1/1	0.98	0.04	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.