Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:12 AM BST

PDB ID	:	2GBC
Title	:	Native DPP-IV (CD26) from Rat
Authors	:	Longenecker, K.L.; Jakob, C.G.; Fry, E.H.; Wilk, S.
Deposited on	:	2006-03-10
Resolution	:	2.80 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:

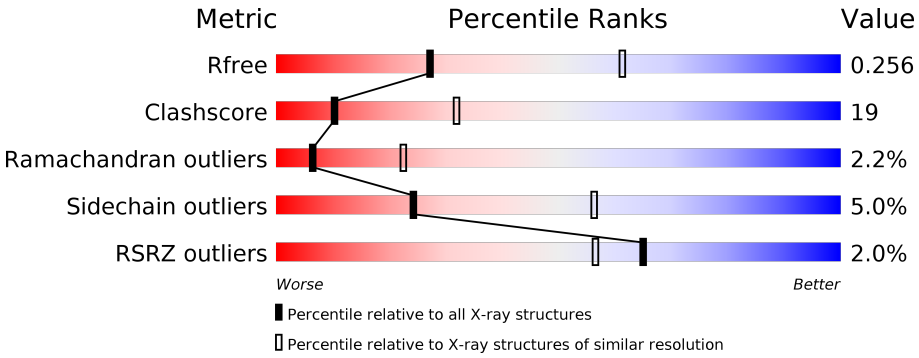
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	730	2% 66% 29% .
1	B	730	2% 67% 28% .

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	1090	X	-	-	-
2	NAG	A	1227	X	-	-	-
2	NAG	B	1083	X	-	-	-
2	NAG	B	1227	X	-	-	-
2	NAG	B	1521	-	-	-	X

2 Entry composition

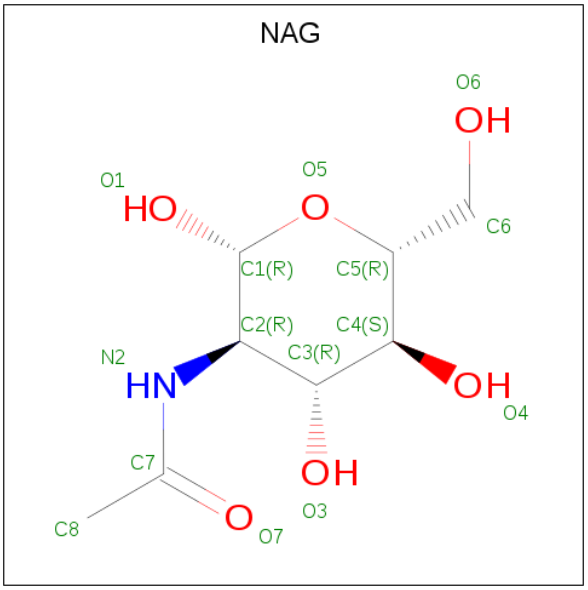
There are 3 unique types of molecules in this entry. The entry contains 12041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5940	3804	983	1127	26			
1	B	730	Total	C	N	O	S	0	0	0
			5940	3804	983	1127	26			

- 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	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

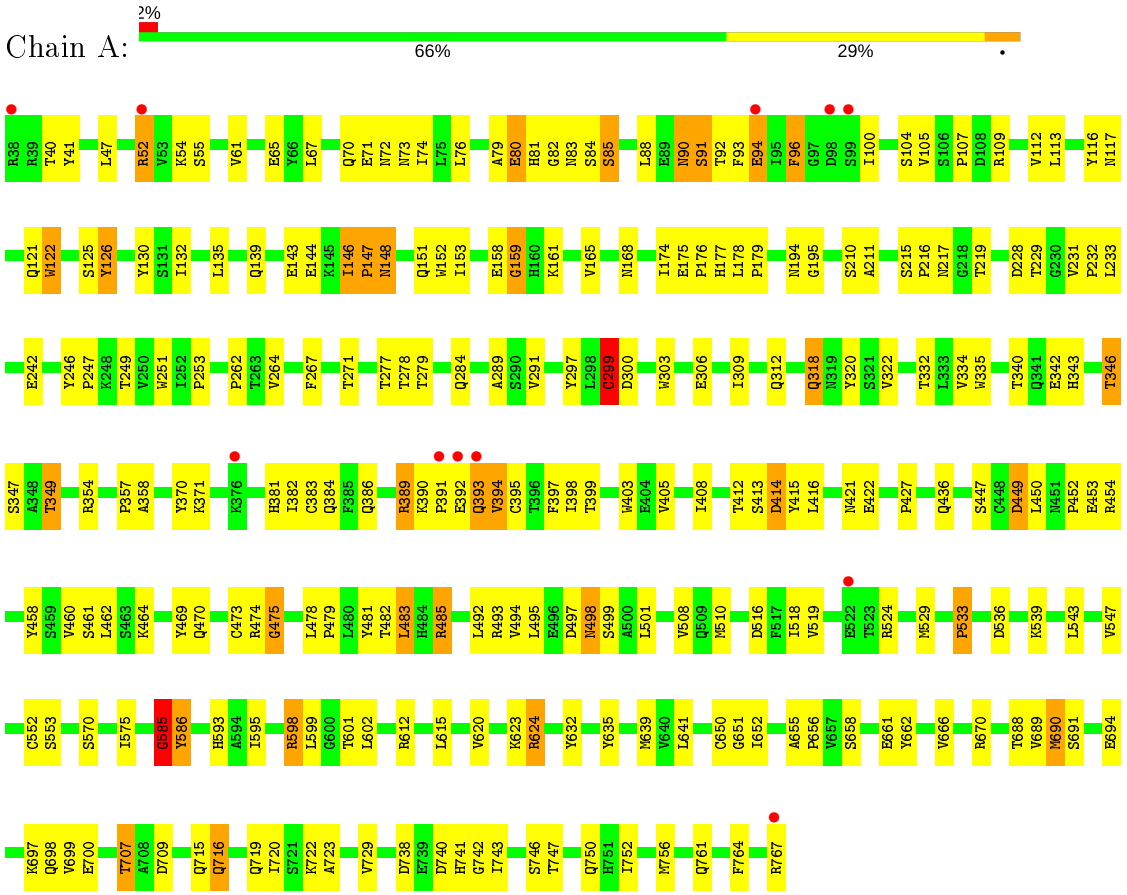
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	11	Total	O	0	0
			11	11		

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.

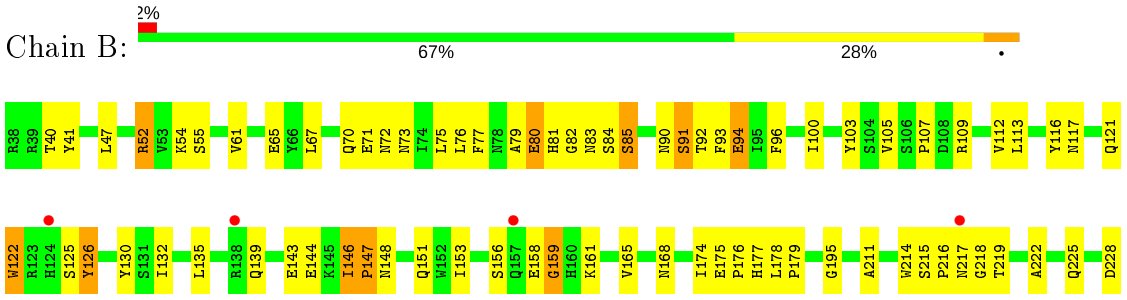
- Molecule 1: Dipeptidyl peptidase 4

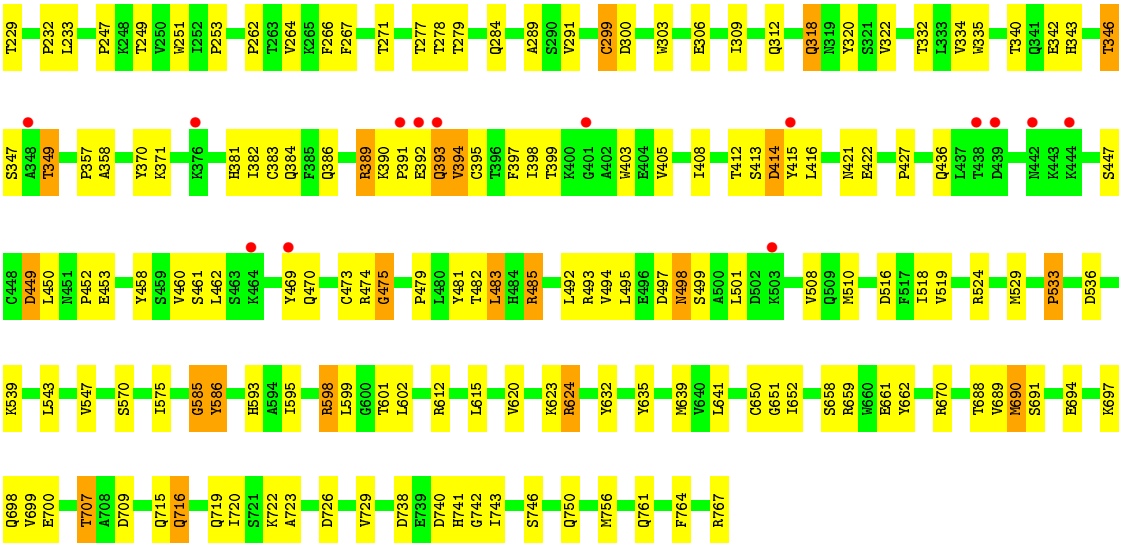
Chain A:



- Molecule 1: Dipeptidyl peptidase 4

Chain B:




T229 P232 L233 P247 K248 T249 V250 W251 I252 P253 P262 T263 V264 K265 F266 F267 T271 T277 T278 T279 Q284 A289 S290 V291 C299 D300 W303 E306 I309 Q312 Q318 N319 Y320 S321 V322 T332 L333 V334 W335 T340 Q341 E342 H343 T346
S347 A348 T349 P357 A358 Y370 K371 K376 H381 I382 C383 Q384 F385 Q386 R389 K390 P391 E392 Q393 V394 C395 T396 F397 I398 T399 K400 Q401 A402 W403 E404 V405 I408 T412 S413 D414 Y415 L416 N421 E422 P427 Q436 L437 T438 D439 N442 K443 K444 S447
C448 D449 L450 N451 P452 E453 Y458 S459 V460 S461 L462 S463 K464 Y469 Q470 C473 R474 G475 P479 L480 Y481 T482 L483 H484 R485 L492 R493 V494 L495 E496 D497 N498 S499 A500 L501 D502 K503 V508 Q509 M510 D516 F517 I518 V519 R524 M529 P533 D536
K539 L543 V547 S570 I575 G585 Y586 H593 A594 I595 R598 L599 G600 T601 L602 R612 L615 V620 K623 R624 Y632 Y635 M639 V640 L641 C650 G651 I652 S658 R659 W660 E661 Y662 R670 T688 V689 M690 S691 E694 K697
Q698 V699 E700 T707 A708 D709 Q715 Q716 Q719 I720 S721 K722 A723 D726 V729 D738 E739 D740 H741 G742 I743 S746 Q750 M756 Q761 F764 R767

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	208.15Å 208.15Å 208.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.80) 98.7 (19.94-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.258 0.228 , 0.256	Depositor DCC
R_{free} test set	3673 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12041	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: NAG

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	0.45	2/6109 (0.0%)	0.71	4/8305 (0.0%)
1	B	0.42	0/6109	0.71	4/8305 (0.0%)
All	All	0.44	2/12218 (0.0%)	0.71	8/16610 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	PHE	CE1-CZ	5.08	1.47	1.37
1	A	299	CYS	CB-SG	-5.02	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	389	ARG	NE-CZ-NH2	-14.79	112.90	120.30
1	B	389	ARG	NE-CZ-NH1	14.20	127.40	120.30
1	A	389	ARG	NE-CZ-NH1	-13.90	113.35	120.30
1	A	389	ARG	NE-CZ-NH2	12.44	126.52	120.30
1	B	389	ARG	CD-NE-CZ	7.24	133.73	123.60
1	A	585	GLY	N-CA-C	6.71	129.88	113.10
1	B	585	GLY	N-CA-C	6.62	129.65	113.10
1	A	389	ARG	CD-NE-CZ	6.38	132.53	123.60

There are no chirality outliers.

There are no planarity outliers.

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	5940	0	5666	221	0
1	B	5940	0	5666	212	0
2	A	70	0	65	8	0
2	B	70	0	65	8	0
3	A	10	0	0	0	0
3	B	11	0	0	0	0
All	All	12041	0	11462	439	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 (439) 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:B:151:GLN:HE22	1:B:168:ASN:H	1.07	0.93
1:A:151:GLN:HE22	1:A:168:ASN:H	1.07	0.93
1:A:412:THR:HG22	1:A:414:ASP:H	1.38	0.89
1:A:658:SER:H	1:A:716:GLN:NE2	1.71	0.88
1:B:688:THR:HG22	1:B:691:SER:H	1.37	0.87
1:A:688:THR:HG22	1:A:691:SER:H	1.38	0.86
1:B:151:GLN:NE2	1:B:168:ASN:H	1.74	0.85
1:B:658:SER:H	1:B:716:GLN:NE2	1.74	0.83
1:A:639:MET:CE	1:A:689:VAL:HA	2.09	0.83
1:B:412:THR:HG22	1:B:414:ASP:H	1.42	0.83
1:A:151:GLN:NE2	1:A:168:ASN:H	1.75	0.83
1:A:349:THR:HB	1:A:593:HIS:CD2	2.14	0.83
1:B:217:ASN:HB2	1:B:306:GLU:OE1	1.78	0.82
1:B:349:THR:HB	1:B:593:HIS:CD2	2.14	0.82
1:A:217:ASN:HB2	1:A:306:GLU:OE1	1.78	0.82
1:A:598:ARG:HE	1:A:601:THR:HG21	1.44	0.82
1:B:598:ARG:HE	1:B:601:THR:HG21	1.45	0.81
1:B:639:MET:CE	1:B:689:VAL:HA	2.10	0.81
1:B:73:ASN:HD21	1:B:90:ASN:ND2	1.78	0.81
1:A:624:ARG:HB2	1:A:624:ARG:HH11	1.48	0.78
1:B:449:ASP:O	1:B:452:PRO:HD3	1.83	0.78
1:B:624:ARG:HB2	1:B:624:ARG:HH11	1.49	0.78
1:B:79:ALA:O	1:B:80:GLU:HB2	1.82	0.78
1:A:54:LYS:H	1:A:498:ASN:HD21	1.33	0.77
1:B:688:THR:CG2	1:B:690:MET:HG2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:H	1:B:498:ASN:HD21	1.33	0.76
1:A:52:ARG:HH11	1:A:52:ARG:HB2	1.50	0.76
1:A:449:ASP:O	1:A:452:PRO:HD3	1.85	0.76
1:A:79:ALA:O	1:A:80:GLU:HB2	1.84	0.76
1:A:73:ASN:HD21	1:A:90:ASN:ND2	1.83	0.76
1:B:174:ILE:HD12	1:B:174:ILE:H	1.51	0.76
1:A:121:GLN:O	1:A:125:SER:HB2	1.85	0.75
1:B:52:ARG:HB2	1:B:52:ARG:HH11	1.50	0.75
1:A:52:ARG:HB2	1:A:52:ARG:NH1	2.02	0.75
1:A:688:THR:CG2	1:A:690:MET:HG2	2.16	0.74
1:B:121:GLN:O	1:B:125:SER:HB2	1.87	0.74
1:A:174:ILE:H	1:A:174:ILE:HD12	1.51	0.73
1:B:96:PHE:CD1	1:B:100:ILE:HD11	2.24	0.73
1:B:690:MET:CE	1:B:720:ILE:HA	2.18	0.73
1:B:52:ARG:NH1	1:B:52:ARG:HB2	2.03	0.72
1:B:601:THR:HG22	1:B:602:LEU:N	2.03	0.72
1:A:601:THR:HG22	1:A:602:LEU:N	2.03	0.72
1:A:482:THR:HG22	1:A:494:VAL:HA	1.72	0.72
1:A:690:MET:CE	1:A:720:ILE:HA	2.19	0.71
1:A:91:SER:HA	1:A:94:GLU:OE1	1.91	0.70
1:B:482:THR:HG22	1:B:494:VAL:HA	1.72	0.70
1:B:54:LYS:N	1:B:498:ASN:HD21	1.89	0.70
1:A:381:HIS:CD2	1:A:399:THR:HG22	2.26	0.70
1:A:349:THR:HB	1:A:593:HIS:HD2	1.55	0.70
1:A:54:LYS:N	1:A:498:ASN:HD21	1.89	0.69
1:B:151:GLN:HE22	1:B:168:ASN:N	1.87	0.69
1:A:658:SER:H	1:A:716:GLN:HE21	1.41	0.69
1:B:349:THR:HB	1:B:593:HIS:HD2	1.55	0.69
1:B:91:SER:O	1:B:93:PHE:N	2.25	0.69
1:B:662:TYR:OH	1:B:719:GLN:HG2	1.92	0.69
1:A:54:LYS:H	1:A:498:ASN:ND2	1.91	0.69
2:B:1083:NAG:O7	2:B:1083:NAG:H3	1.92	0.68
1:A:91:SER:O	1:A:93:PHE:N	2.26	0.68
1:B:386:GLN:HG3	1:B:390:LYS:NZ	2.09	0.68
1:B:91:SER:HA	1:B:94:GLU:OE1	1.94	0.68
1:A:662:TYR:OH	1:A:719:GLN:HG2	1.94	0.68
1:A:105:VAL:HG22	1:A:112:VAL:HG22	1.76	0.67
1:A:175:GLU:HB3	1:A:178:LEU:HG	1.76	0.67
1:B:688:THR:HG23	1:B:690:MET:HG2	1.75	0.67
1:A:688:THR:HG23	1:A:690:MET:HG2	1.77	0.67
1:B:175:GLU:HB3	1:B:178:LEU:HG	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:H	1:B:498:ASN:ND2	1.92	0.67
1:A:151:GLN:HE22	1:A:168:ASN:N	1.87	0.66
1:A:586:TYR:CD1	1:A:586:TYR:N	2.63	0.66
1:B:105:VAL:HG22	1:B:112:VAL:HG22	1.76	0.66
1:B:125:SER:O	1:B:126:TYR:HB3	1.95	0.66
1:B:595:ILE:CG2	1:B:599:LEU:HD23	2.26	0.66
1:A:460:VAL:HG22	1:A:461:SER:N	2.10	0.66
1:A:125:SER:O	1:A:126:TYR:HB3	1.96	0.66
1:A:382:ILE:HG13	1:A:405:VAL:HG21	1.78	0.66
1:B:460:VAL:HG22	1:B:461:SER:N	2.11	0.66
1:A:96:PHE:CD1	1:A:100:ILE:HD11	2.30	0.66
1:A:386:GLN:HG3	1:A:390:LYS:NZ	2.10	0.65
1:A:595:ILE:CG2	1:A:599:LEU:HD23	2.26	0.65
1:A:370:TYR:CE2	1:A:384:GLN:HG3	2.31	0.65
1:B:392:GLU:C	1:B:393:GLN:HG3	2.17	0.65
1:B:277:THR:HG21	1:B:279:THR:O	1.97	0.65
1:A:624:ARG:HB2	1:A:624:ARG:NH1	2.11	0.65
1:B:146:ILE:HD12	1:B:153:ILE:HD12	1.79	0.64
1:B:586:TYR:N	1:B:586:TYR:CD1	2.64	0.64
1:A:277:THR:HG21	1:A:279:THR:O	1.97	0.64
1:B:658:SER:H	1:B:716:GLN:HE21	1.45	0.64
1:A:392:GLU:C	1:A:393:GLN:HG3	2.16	0.64
1:A:146:ILE:HD12	1:A:153:ILE:HD12	1.80	0.64
1:B:624:ARG:NH1	1:B:624:ARG:HB2	2.12	0.64
1:A:639:MET:HE3	1:A:689:VAL:HA	1.80	0.63
1:A:719:GLN:NE2	1:A:722:LYS:HE2	2.13	0.63
1:A:52:ARG:HH11	1:A:52:ARG:CB	2.12	0.62
1:B:381:HIS:CD2	1:B:399:THR:HG22	2.33	0.62
1:B:719:GLN:NE2	1:B:722:LYS:HE2	2.14	0.62
1:A:694:GLU:O	1:A:697:LYS:HG3	2.00	0.62
1:B:370:TYR:CE2	1:B:384:GLN:HG3	2.34	0.62
1:B:52:ARG:CB	1:B:52:ARG:HH11	2.12	0.62
1:B:81:HIS:O	1:B:83:ASN:N	2.32	0.62
1:B:612:ARG:HH11	1:B:612:ARG:HG3	1.65	0.62
1:B:79:ALA:O	1:B:80:GLU:CB	2.48	0.62
1:B:382:ILE:HG13	1:B:405:VAL:HG21	1.82	0.61
1:B:389:ARG:HG3	1:B:394:VAL:HG13	1.82	0.61
1:A:174:ILE:HD12	1:A:174:ILE:N	2.15	0.61
1:A:612:ARG:HH11	1:A:612:ARG:HG3	1.65	0.61
1:B:694:GLU:O	1:B:697:LYS:HG3	2.01	0.61
1:A:79:ALA:O	1:A:80:GLU:CB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ASN:HB3	1:B:501:LEU:HB3	1.83	0.60
1:B:383:CYS:HB3	1:B:397:PHE:CD2	2.37	0.60
1:B:174:ILE:HD12	1:B:174:ILE:N	2.17	0.60
1:A:81:HIS:O	1:A:83:ASN:N	2.34	0.60
1:B:65:GLU:HB3	1:B:76:LEU:HD11	1.84	0.60
1:A:529:MET:HE2	1:A:575:ILE:HG21	1.83	0.60
1:B:299:CYS:SG	1:B:357:PRO:HD2	2.42	0.60
1:B:412:THR:CG2	1:B:413:SER:N	2.64	0.60
1:A:485:ARG:HG3	1:A:485:ARG:O	2.00	0.60
1:A:641:LEU:HD22	1:A:699:VAL:HG11	1.83	0.60
1:B:55:SER:HA	1:B:481:TYR:CE1	2.37	0.60
1:B:81:HIS:C	1:B:83:ASN:H	2.05	0.60
1:A:146:ILE:HG13	1:A:147:PRO:HD2	1.82	0.59
1:A:65:GLU:HB3	1:A:76:LEU:HD11	1.83	0.59
1:B:146:ILE:HG13	1:B:147:PRO:HD2	1.83	0.59
1:B:412:THR:HG22	1:B:413:SER:N	2.16	0.59
1:B:229:THR:HG21	2:B:1227:NAG:H62	1.85	0.59
1:B:485:ARG:HG3	1:B:485:ARG:O	2.01	0.59
1:A:412:THR:CG2	1:A:413:SER:N	2.66	0.59
1:B:697:LYS:HG2	1:B:729:VAL:HG22	1.85	0.58
1:A:55:SER:HA	1:A:481:TYR:CE1	2.39	0.58
1:B:639:MET:HE3	1:B:689:VAL:HA	1.85	0.58
1:A:498:ASN:HB3	1:A:501:LEU:HB3	1.85	0.58
1:A:383:CYS:HB3	1:A:397:PHE:CD2	2.39	0.58
1:A:158:GLU:OE1	1:A:217:ASN:HA	2.04	0.58
1:A:381:HIS:CD2	1:A:399:THR:CG2	2.86	0.57
1:A:697:LYS:HG2	1:A:729:VAL:HG22	1.86	0.57
1:B:483:LEU:HB3	1:B:495:LEU:HD11	1.85	0.57
1:A:158:GLU:HG3	1:A:159:GLY:H	1.70	0.57
1:A:299:CYS:SG	1:A:357:PRO:HD2	2.45	0.57
1:A:107:PRO:HG2	1:A:158:GLU:O	2.05	0.56
1:A:408:ILE:HG23	1:A:416:LEU:HD11	1.87	0.56
1:B:158:GLU:OE1	1:B:217:ASN:HA	2.05	0.56
1:B:233:LEU:HD13	1:B:251:TRP:HE3	1.70	0.56
1:B:408:ILE:HG23	1:B:416:LEU:HD11	1.87	0.56
1:B:146:ILE:CD1	1:B:153:ILE:HD12	2.36	0.56
1:B:175:GLU:HB3	1:B:178:LEU:CG	2.36	0.56
1:B:460:VAL:HG22	1:B:461:SER:H	1.70	0.56
1:A:41:TYR:HB2	1:A:510:MET:HE1	1.87	0.56
1:B:277:THR:HG22	1:B:279:THR:H	1.70	0.56
1:B:497:ASP:O	1:B:499:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:THR:HG22	1:A:602:LEU:H	1.68	0.56
1:A:81:HIS:C	1:A:83:ASN:H	2.07	0.56
1:A:598:ARG:HD3	1:A:598:ARG:O	2.06	0.56
1:A:715:GLN:NE2	1:B:247:PRO:HD3	2.21	0.56
1:B:195:GLY:C	1:B:211:ALA:HB3	2.26	0.55
1:A:460:VAL:HG22	1:A:461:SER:H	1.70	0.55
1:A:497:ASP:O	1:A:499:SER:N	2.37	0.55
1:A:688:THR:HG22	1:A:691:SER:N	2.17	0.55
1:A:41:TYR:HB2	1:A:510:MET:CE	2.36	0.55
1:B:158:GLU:HG3	1:B:159:GLY:H	1.72	0.55
1:B:543:LEU:HD12	1:B:575:ILE:O	2.07	0.55
1:A:412:THR:HG22	1:A:413:SER:N	2.19	0.55
1:A:707:THR:CG2	1:A:738:ASP:H	2.19	0.55
1:B:47:LEU:HD22	1:B:750:GLN:HA	1.87	0.55
1:B:41:TYR:HB2	1:B:510:MET:HE1	1.88	0.55
1:A:175:GLU:HB3	1:A:178:LEU:CG	2.36	0.55
1:A:543:LEU:HD12	1:A:575:ILE:O	2.07	0.55
1:A:332:THR:O	1:A:334:VAL:HG23	2.07	0.55
1:A:598:ARG:NE	1:A:601:THR:HG21	2.19	0.55
1:B:389:ARG:HG3	1:B:394:VAL:CG1	2.36	0.55
1:B:641:LEU:HD22	1:B:699:VAL:HG11	1.88	0.55
1:B:529:MET:HE3	1:B:575:ILE:HG21	1.88	0.55
1:A:358:ALA:O	1:A:371:LYS:HE3	2.07	0.54
1:A:641:LEU:HD11	1:A:651:GLY:HA3	1.88	0.54
2:B:1083:NAG:O7	2:B:1083:NAG:C3	2.54	0.54
1:A:146:ILE:CD1	1:A:153:ILE:HD12	2.37	0.54
1:A:447:SER:HB2	1:A:458:TYR:CE1	2.42	0.54
1:B:41:TYR:HB2	1:B:510:MET:CE	2.36	0.54
2:B:1227:NAG:O7	2:B:1227:NAG:C3	2.56	0.54
1:B:109:ARG:O	1:B:135:LEU:HD12	2.08	0.54
1:A:195:GLY:C	1:A:211:ALA:HB3	2.28	0.54
1:B:175:GLU:HG3	1:B:177:HIS:H	1.72	0.54
1:B:267:PHE:CE2	1:B:284:GLN:HB2	2.43	0.54
1:A:229:THR:HG21	2:A:1227:NAG:H61	1.88	0.54
1:B:346:THR:HG23	1:B:347:SER:N	2.23	0.54
1:B:707:THR:CG2	1:B:738:ASP:H	2.21	0.54
1:B:529:MET:CE	1:B:575:ILE:HG21	2.38	0.54
1:B:598:ARG:HD3	1:B:598:ARG:O	2.08	0.54
1:A:47:LEU:HD22	1:A:750:GLN:HA	1.90	0.53
1:A:277:THR:HG22	1:A:279:THR:H	1.73	0.53
1:B:601:THR:HG22	1:B:602:LEU:H	1.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:GLN:HB3	1:A:767:ARG:HB2	1.91	0.53
1:B:107:PRO:HG2	1:B:158:GLU:O	2.08	0.53
1:B:175:GLU:HB3	1:B:178:LEU:CD1	2.39	0.53
1:B:447:SER:HB2	1:B:458:TYR:CE1	2.44	0.53
1:A:228:ASP:OD1	1:A:262:PRO:HB3	2.08	0.53
1:A:483:LEU:HB3	1:A:495:LEU:HD11	1.89	0.53
1:B:508:VAL:HG12	1:B:510:MET:HE2	1.90	0.53
1:A:233:LEU:HD13	1:A:251:TRP:HE3	1.74	0.53
1:A:383:CYS:HB3	1:A:397:PHE:HA	1.90	0.53
1:A:690:MET:HB3	1:A:723:ALA:HB2	1.90	0.53
1:B:474:ARG:O	1:B:475:GLY:O	2.26	0.53
1:B:358:ALA:O	1:B:371:LYS:HE3	2.08	0.53
2:B:1090:NAG:H3	2:B:1090:NAG:O7	2.09	0.53
1:B:249:THR:CG2	1:B:251:TRP:HE1	2.22	0.53
1:B:96:PHE:HB2	1:B:100:ILE:HG12	1.91	0.53
1:A:175:GLU:HG3	1:A:177:HIS:H	1.72	0.52
1:B:381:HIS:CD2	1:B:399:THR:CG2	2.91	0.52
1:A:267:PHE:CE2	1:A:284:GLN:HB2	2.43	0.52
1:A:529:MET:CE	1:A:575:ILE:HG21	2.39	0.52
1:B:84:SER:O	1:B:85:SER:HB2	2.09	0.52
1:B:219:THR:O	1:B:271:THR:HB	2.10	0.52
1:B:462:LEU:N	1:B:462:LEU:HD12	2.24	0.52
1:A:109:ARG:O	1:A:135:LEU:HD12	2.08	0.52
1:B:334:VAL:HG12	1:B:335:TRP:N	2.24	0.52
1:A:132:ILE:HG21	1:A:176:PRO:HB3	1.91	0.52
1:B:641:LEU:HD11	1:B:651:GLY:HA3	1.91	0.52
1:A:175:GLU:HB3	1:A:178:LEU:CD1	2.40	0.52
1:A:346:THR:HG23	1:A:347:SER:N	2.25	0.52
1:B:403:TRP:CE3	1:B:422:GLU:HB2	2.45	0.52
1:A:415:TYR:HD2	1:A:436:GLN:HA	1.74	0.52
1:B:81:HIS:C	1:B:83:ASN:N	2.63	0.51
1:A:70:GLN:HG2	1:A:71:GLU:HG3	1.91	0.51
1:B:96:PHE:CG	1:B:100:ILE:HD11	2.45	0.51
1:B:217:ASN:CB	1:B:306:GLU:OE1	2.55	0.51
1:A:219:THR:O	1:A:271:THR:HB	2.11	0.51
1:B:132:ILE:HG21	1:B:176:PRO:HB3	1.91	0.51
1:B:332:THR:O	1:B:334:VAL:HG23	2.11	0.51
1:B:473:CYS:O	1:B:479:PRO:HA	2.11	0.51
1:B:598:ARG:NE	1:B:601:THR:HG21	2.21	0.51
1:A:96:PHE:HB2	1:A:100:ILE:HG12	1.92	0.51
1:B:639:MET:HE1	1:B:689:VAL:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLN:HG2	1:B:71:GLU:HG3	1.91	0.51
1:A:84:SER:O	1:A:85:SER:HB2	2.11	0.51
1:A:229:THR:HG21	2:A:1227:NAG:C6	2.40	0.50
1:A:473:CYS:O	1:A:479:PRO:HA	2.11	0.50
1:B:116:TYR:O	1:B:117:ASN:HB2	2.10	0.50
1:B:485:ARG:HB3	1:B:492:LEU:HD21	1.93	0.50
1:B:415:TYR:HD2	1:B:436:GLN:HA	1.75	0.50
1:A:747:THR:HG21	1:B:726:ASP:HA	1.94	0.50
1:B:225:GLN:OE1	2:B:1227:NAG:H83	2.11	0.50
1:B:632:TYR:O	1:B:635:TYR:HB3	2.12	0.50
1:A:40:THR:HB	1:A:570:SER:OG	2.11	0.50
1:A:61:VAL:CG2	1:A:67:LEU:HG	2.41	0.50
1:A:81:HIS:C	1:A:83:ASN:N	2.65	0.50
1:B:228:ASP:OD1	1:B:262:PRO:HB3	2.11	0.50
1:A:389:ARG:HG3	1:A:394:VAL:CG1	2.42	0.50
1:B:690:MET:HB3	1:B:723:ALA:HB2	1.93	0.50
1:B:761:GLN:HB3	1:B:767:ARG:HB2	1.94	0.50
1:A:116:TYR:O	1:A:117:ASN:HB2	2.12	0.49
1:A:474:ARG:O	1:A:475:GLY:O	2.29	0.49
1:B:383:CYS:HB3	1:B:397:PHE:HA	1.93	0.49
1:A:508:VAL:HG12	1:A:510:MET:HE2	1.94	0.49
2:B:1521:NAG:H3	2:B:1521:NAG:O7	2.11	0.49
1:A:242:GLU:HG3	1:B:659:ARG:NH1	2.28	0.49
1:B:688:THR:HG22	1:B:691:SER:N	2.17	0.49
1:A:650:CYS:HB3	1:A:700:GLU:HB2	1.94	0.49
1:A:122:TRP:CE3	1:A:122:TRP:N	2.81	0.49
1:A:334:VAL:HG12	1:A:335:TRP:N	2.27	0.49
1:A:632:TYR:O	1:A:635:TYR:HB3	2.13	0.49
1:A:247:PRO:HD3	1:B:715:GLN:NE2	2.27	0.49
1:B:318:GLN:NE2	1:B:670:ARG:HB2	2.28	0.49
1:B:40:THR:HB	1:B:570:SER:OG	2.13	0.49
1:B:122:TRP:N	1:B:122:TRP:CE3	2.81	0.48
1:A:299:CYS:HB2	1:A:312:GLN:O	2.13	0.48
1:A:688:THR:HG21	1:A:690:MET:HG2	1.94	0.48
1:A:144:GLU:HG3	1:A:179:PRO:N	2.28	0.48
1:A:403:TRP:CE3	1:A:422:GLU:HB2	2.49	0.48
1:A:462:LEU:N	1:A:462:LEU:HD12	2.28	0.48
1:A:249:THR:CG2	1:A:251:TRP:HE1	2.26	0.48
1:A:343:HIS:HA	1:A:389:ARG:HD2	1.95	0.48
1:A:61:VAL:CG1	1:A:109:ARG:NE	2.77	0.48
1:A:601:THR:HG22	1:A:602:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLU:O	1:B:306:GLU:HG3	2.13	0.48
1:B:61:VAL:CG1	1:B:109:ARG:NE	2.77	0.48
1:A:217:ASN:CB	1:A:306:GLU:OE1	2.56	0.48
1:A:624:ARG:HG2	1:A:764:PHE:CD2	2.49	0.48
1:A:460:VAL:CG2	1:A:461:SER:N	2.75	0.48
1:A:96:PHE:CG	1:A:100:ILE:HD11	2.48	0.48
1:B:61:VAL:CG2	1:B:67:LEU:HG	2.43	0.48
1:B:690:MET:CE	1:B:720:ILE:CA	2.91	0.48
1:B:277:THR:HG22	1:B:278:THR:N	2.29	0.47
1:B:624:ARG:HG2	1:B:764:PHE:CD2	2.49	0.47
1:B:650:CYS:HB3	1:B:700:GLU:HB2	1.96	0.47
1:A:536:ASP:HB3	1:A:539:LYS:NZ	2.29	0.47
1:B:175:GLU:HB3	1:B:178:LEU:HD12	1.96	0.47
1:A:277:THR:CG2	1:A:279:THR:O	2.62	0.47
1:A:421:ASN:ND2	1:A:427:PRO:HA	2.29	0.47
1:B:61:VAL:HG11	1:B:109:ARG:NE	2.29	0.47
1:A:130:TYR:HB2	1:A:146:ILE:HD13	1.97	0.47
1:B:601:THR:CG2	1:B:602:LEU:N	2.70	0.47
1:B:688:THR:HG21	1:B:690:MET:HG2	1.93	0.47
1:A:485:ARG:HB3	1:A:492:LEU:HD21	1.96	0.47
1:B:174:ILE:H	1:B:174:ILE:CD1	2.23	0.47
1:A:61:VAL:HG11	1:A:109:ARG:NE	2.30	0.47
1:B:460:VAL:CG2	1:B:461:SER:N	2.76	0.47
1:A:306:GLU:HG3	1:A:306:GLU:O	2.15	0.47
1:B:144:GLU:HG3	1:B:179:PRO:N	2.28	0.47
1:A:175:GLU:HB3	1:A:178:LEU:HD12	1.97	0.47
1:A:383:CYS:CB	1:A:397:PHE:HA	2.46	0.46
1:A:80:GLU:H	1:A:493:ARG:HH22	1.63	0.46
1:A:389:ARG:HG3	1:A:394:VAL:HG13	1.96	0.46
1:A:454:ARG:HD3	1:A:478:LEU:O	2.16	0.46
1:B:346:THR:CG2	1:B:347:SER:N	2.79	0.46
1:A:639:MET:HE1	1:A:689:VAL:HA	1.93	0.46
1:A:746:SER:O	1:A:750:GLN:HG3	2.16	0.46
1:A:518:ILE:CG2	1:A:519:VAL:N	2.79	0.46
1:A:612:ARG:NH1	1:A:612:ARG:HG3	2.31	0.46
1:B:398:ILE:HG22	1:B:398:ILE:O	2.15	0.46
1:B:742:GLY:O	1:B:743:ILE:C	2.54	0.46
2:A:1521:NAG:O7	2:A:1521:NAG:H3	2.16	0.46
1:A:460:VAL:CG2	1:A:461:SER:H	2.29	0.46
1:A:318:GLN:NE2	1:A:670:ARG:HB2	2.31	0.45
1:A:174:ILE:H	1:A:174:ILE:CD1	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HB3	1:A:179:PRO:HD2	1.98	0.45
2:A:1083:NAG:O7	2:A:1083:NAG:H3	2.15	0.45
2:A:1227:NAG:O7	2:A:1227:NAG:C3	2.64	0.45
1:A:233:LEU:HD23	1:A:253:PRO:HA	1.98	0.45
1:A:639:MET:HE3	1:A:689:VAL:CA	2.45	0.45
1:B:277:THR:CG2	1:B:279:THR:O	2.64	0.45
1:B:421:ASN:ND2	1:B:427:PRO:HA	2.31	0.45
1:B:746:SER:O	1:B:750:GLN:HG3	2.17	0.45
1:A:151:GLN:NE2	1:A:165:VAL:HG12	2.32	0.45
1:A:346:THR:CG2	1:A:347:SER:N	2.80	0.45
1:A:709:ASP:OD2	1:A:741:HIS:HA	2.16	0.45
1:B:61:VAL:HG21	1:B:67:LEU:HG	1.99	0.45
1:A:61:VAL:HG21	1:A:67:LEU:HG	1.98	0.45
1:B:93:PHE:O	1:B:100:ILE:HG13	2.17	0.45
1:B:299:CYS:HB2	1:B:312:GLN:O	2.17	0.45
1:B:399:THR:CG2	1:B:403:TRP:CH2	3.00	0.45
1:B:460:VAL:CG2	1:B:461:SER:H	2.30	0.45
1:A:398:ILE:HG22	1:A:398:ILE:O	2.16	0.44
1:B:612:ARG:HG3	1:B:612:ARG:NH1	2.30	0.44
1:B:289:ALA:C	1:B:291:VAL:H	2.21	0.44
1:B:412:THR:CG2	1:B:413:SER:H	2.29	0.44
1:B:518:ILE:CG2	1:B:519:VAL:N	2.79	0.44
1:B:690:MET:HE2	1:B:720:ILE:HA	1.99	0.44
1:A:386:GLN:HG3	1:A:390:LYS:HZ1	1.81	0.44
1:A:740:ASP:OD1	1:A:741:HIS:N	2.43	0.44
1:B:690:MET:HB3	1:B:723:ALA:CB	2.47	0.44
1:B:84:SER:O	1:B:85:SER:CB	2.66	0.44
1:A:497:ASP:O	1:A:497:ASP:CG	2.55	0.44
1:A:342:GLU:O	1:A:389:ARG:HD3	2.17	0.44
1:A:690:MET:HB3	1:A:723:ALA:CB	2.46	0.44
1:A:412:THR:CG2	1:A:413:SER:H	2.31	0.44
1:A:415:TYR:CD2	1:A:436:GLN:HA	2.52	0.44
1:B:536:ASP:HB3	1:B:539:LYS:NZ	2.33	0.44
1:B:709:ASP:OD2	1:B:741:HIS:HA	2.18	0.44
1:A:229:THR:HB	2:A:1227:NAG:H62	1.98	0.44
1:A:148:ASN:HD22	1:A:148:ASN:HA	1.58	0.44
1:B:233:LEU:HD23	1:B:253:PRO:HA	2.00	0.44
1:B:383:CYS:CB	1:B:397:PHE:HA	2.47	0.44
1:B:71:GLU:O	1:B:72:ASN:HB2	2.17	0.44
1:A:84:SER:O	1:A:85:SER:CB	2.67	0.43
1:B:215:SER:HB3	1:B:303:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:LYS:HD3	1:B:623:LYS:HA	1.88	0.43
1:B:615:LEU:HD23	1:B:620:VAL:CG1	2.48	0.43
1:B:403:TRP:CD2	1:B:422:GLU:HB2	2.54	0.43
1:B:652:ILE:HG21	1:B:756:MET:HE2	1.99	0.43
2:A:1521:NAG:O7	2:A:1521:NAG:C3	2.67	0.43
1:B:249:THR:HG21	1:B:251:TRP:HE1	1.82	0.43
1:B:233:LEU:CD1	1:B:251:TRP:HE3	2.31	0.43
1:A:652:ILE:HG21	1:A:756:MET:HE2	1.99	0.43
1:A:690:MET:CE	1:A:720:ILE:CA	2.93	0.43
1:A:71:GLU:O	1:A:72:ASN:HB2	2.18	0.43
1:A:277:THR:HG22	1:A:278:THR:N	2.33	0.43
1:A:469:TYR:O	1:A:469:TYR:CD1	2.72	0.43
1:B:130:TYR:HB2	1:B:146:ILE:HD13	2.00	0.43
1:B:639:MET:HE3	1:B:689:VAL:CA	2.49	0.43
1:B:303:TRP:CE2	1:B:309:ILE:HD12	2.54	0.42
1:A:639:MET:CE	1:A:689:VAL:HG22	2.49	0.42
1:B:151:GLN:NE2	1:B:165:VAL:HG12	2.33	0.42
1:B:222:ALA:HB1	1:B:266:PHE:CZ	2.53	0.42
1:B:415:TYR:CD2	1:B:436:GLN:HA	2.54	0.42
1:A:623:LYS:HA	1:A:623:LYS:HD3	1.85	0.42
1:A:742:GLY:O	1:A:743:ILE:C	2.57	0.42
1:A:615:LEU:HD23	1:A:620:VAL:CG1	2.50	0.42
1:A:246:TYR:CZ	1:B:232:PRO:HB2	2.54	0.42
1:B:740:ASP:OD1	1:B:741:HIS:N	2.41	0.42
1:A:399:THR:CG2	1:A:403:TRP:CH2	3.03	0.42
1:A:553:SER:O	1:A:585:GLY:N	2.48	0.42
1:A:93:PHE:O	1:A:100:ILE:HG13	2.19	0.42
1:A:343:HIS:ND1	1:A:394:VAL:HG11	2.34	0.42
1:A:761:GLN:HB3	1:A:767:ARG:H	1.83	0.42
1:B:320:TYR:CE2	1:B:322:VAL:HG23	2.54	0.42
1:A:168:ASN:O	1:A:194:ASN:HB2	2.19	0.42
1:B:322:VAL:CG1	1:B:342:GLU:HG2	2.49	0.42
1:B:343:HIS:ND1	1:B:394:VAL:HG11	2.35	0.42
1:B:91:SER:HA	1:B:94:GLU:CD	2.39	0.42
1:A:289:ALA:C	1:A:291:VAL:H	2.23	0.42
1:A:690:MET:HE1	1:A:720:ILE:CG1	2.50	0.42
1:B:497:ASP:CG	1:B:497:ASP:O	2.58	0.42
1:B:601:THR:HG22	1:B:602:LEU:HD23	2.02	0.42
1:A:303:TRP:CE2	1:A:309:ILE:HD12	2.54	0.42
1:B:156:SER:HA	1:B:214:TRP:CD1	2.55	0.42
1:A:529:MET:HE2	1:A:575:ILE:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ILE:HD13	1:A:595:ILE:HA	1.81	0.41
1:A:74:ILE:HB	1:A:88:LEU:HB2	2.02	0.41
1:B:601:THR:CG2	1:B:602:LEU:H	2.28	0.41
1:A:233:LEU:CD1	1:A:251:TRP:HE3	2.34	0.41
1:A:403:TRP:CD2	1:A:422:GLU:HB2	2.55	0.41
1:A:524:ARG:HG2	1:A:524:ARG:HH11	1.85	0.41
1:A:752:ILE:O	1:A:756:MET:HG3	2.20	0.41
1:B:161:LYS:HG2	1:B:174:ILE:HA	2.01	0.41
1:A:231:VAL:HA	1:A:232:PRO:HD3	1.93	0.41
1:A:320:TYR:CE2	1:A:322:VAL:HG23	2.55	0.41
1:B:216:PRO:O	1:B:217:ASN:HB2	2.20	0.41
1:B:518:ILE:HA	1:B:518:ILE:HD13	1.89	0.41
1:A:464:LYS:HA	1:A:464:LYS:HD3	1.87	0.41
1:A:655:ALA:N	1:A:656:PRO:CD	2.84	0.41
1:B:103:TYR:HA	1:B:113:LEU:O	2.20	0.41
1:B:80:GLU:H	1:B:493:ARG:HH22	1.67	0.41
1:B:216:PRO:O	1:B:306:GLU:OE2	2.39	0.41
1:B:659:ARG:HG2	1:B:662:TYR:CE2	2.55	0.41
1:B:639:MET:HE3	1:B:689:VAL:CG2	2.51	0.41
1:B:75:LEU:HB2	1:B:77:PHE:HE1	1.85	0.41
1:B:96:PHE:HB2	1:B:100:ILE:CG1	2.51	0.41
1:A:354:ARG:HD3	1:A:552:CYS:SG	2.60	0.41
1:A:601:THR:CG2	1:A:602:LEU:N	2.69	0.41
1:B:343:HIS:HA	1:B:389:ARG:HD3	2.02	0.41
1:B:639:MET:CE	1:B:689:VAL:HG22	2.51	0.41
1:A:152:TRP:CE2	1:A:210:SER:HB2	2.56	0.41
1:A:216:PRO:O	1:A:306:GLU:OE2	2.39	0.41
1:A:91:SER:HA	1:A:94:GLU:CD	2.41	0.41
1:B:524:ARG:HH11	1:B:524:ARG:HG2	1.85	0.41
1:A:322:VAL:CG1	1:A:342:GLU:HG2	2.51	0.40
1:B:178:LEU:HB3	1:B:179:PRO:HD2	2.01	0.40
1:B:469:TYR:O	1:B:469:TYR:CD1	2.74	0.40
1:B:690:MET:HE1	1:B:720:ILE:CG1	2.50	0.40
1:B:73:ASN:HD21	1:B:90:ASN:CG	2.21	0.40
1:A:104:SER:HB3	1:A:113:LEU:HB2	2.04	0.40
1:A:73:ASN:HD21	1:A:90:ASN:CG	2.23	0.40
2:A:1227:NAG:H3	2:A:1227:NAG:O7	2.21	0.40
1:A:215:SER:HB3	1:A:303:TRP:CZ2	2.56	0.40
1:A:297:TYR:CE2	1:A:666:VAL:HG22	2.56	0.40
1:A:586:TYR:H	1:A:586:TYR:HD1	1.68	0.40
1:A:601:THR:CG2	1:A:602:LEU:H	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1227:NAG:O7	2:B:1227:NAG:O3	2.37	0.40
1:B:161:LYS:NZ	1:B:218:GLY:O	2.52	0.40
1:A:161:LYS:HG2	1:A:174:ILE:HA	2.03	0.40
1:A:175:GLU:OE2	1:A:176:PRO:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	728/730 (100%)	645 (89%)	67 (9%)	16 (2%)	6 22
1	B	728/730 (100%)	647 (89%)	65 (9%)	16 (2%)	6 22
All	All	1456/1460 (100%)	1292 (89%)	132 (9%)	32 (2%)	6 22

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	475	GLY
1	A	533	PRO
1	A	585	GLY
1	B	80	GLU
1	B	475	GLY
1	B	533	PRO
1	B	585	GLY
1	A	82	GLY
1	A	85	SER
1	A	91	SER
1	A	126	TYR
1	A	143	GLU
1	A	450	LEU

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Mol	Chain	Res	Type
1	A	498	ASN
1	B	82	GLY
1	B	85	SER
1	B	91	SER
1	B	126	TYR
1	B	143	GLU
1	B	450	LEU
1	B	318	GLN
1	B	498	ASN
1	A	92	THR
1	A	318	GLN
1	B	92	THR
1	A	147	PRO
1	B	147	PRO
1	B	391	PRO
1	A	391	PRO
1	A	159	GLY
1	B	159	GLY

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	649/651 (100%)	616 (95%)	33 (5%)	24	55
1	B	649/651 (100%)	617 (95%)	32 (5%)	25	57
All	All	1298/1302 (100%)	1233 (95%)	65 (5%)	24	56

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	90	ASN
1	A	94	GLU
1	A	122	TRP
1	A	139	GLN

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Mol	Chain	Res	Type
1	A	146	ILE
1	A	148	ASN
1	A	264	VAL
1	A	299	CYS
1	A	300	ASP
1	A	340	THR
1	A	346	THR
1	A	349	THR
1	A	393	GLN
1	A	394	VAL
1	A	395	CYS
1	A	414	ASP
1	A	449	ASP
1	A	453	GLU
1	A	470	GLN
1	A	483	LEU
1	A	485	ARG
1	A	516	ASP
1	A	533	PRO
1	A	547	VAL
1	A	586	TYR
1	A	598	ARG
1	A	624	ARG
1	A	661	GLU
1	A	690	MET
1	A	698	GLN
1	A	707	THR
1	A	716	GLN
1	B	52	ARG
1	B	94	GLU
1	B	122	TRP
1	B	139	GLN
1	B	146	ILE
1	B	148	ASN
1	B	264	VAL
1	B	299	CYS
1	B	300	ASP
1	B	340	THR
1	B	346	THR
1	B	349	THR
1	B	393	GLN
1	B	394	VAL

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Mol	Chain	Res	Type
1	B	395	CYS
1	B	414	ASP
1	B	449	ASP
1	B	453	GLU
1	B	470	GLN
1	B	483	LEU
1	B	485	ARG
1	B	516	ASP
1	B	533	PRO
1	B	547	VAL
1	B	586	TYR
1	B	598	ARG
1	B	624	ARG
1	B	661	GLU
1	B	690	MET
1	B	698	GLN
1	B	707	THR
1	B	716	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	148	ASN
1	A	151	GLN
1	A	341	GLN
1	A	381	HIS
1	A	386	GLN
1	A	470	GLN
1	A	484	HIS
1	A	498	ASN
1	A	593	HIS
1	A	698	GLN
1	A	716	GLN
1	A	719	GLN
1	A	749	HIS
1	A	758	HIS
1	B	73	ASN
1	B	148	ASN
1	B	151	GLN
1	B	341	GLN
1	B	381	HIS

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Mol	Chain	Res	Type
1	B	386	GLN
1	B	470	GLN
1	B	484	HIS
1	B	498	ASN
1	B	593	HIS
1	B	698	GLN
1	B	716	GLN
1	B	719	GLN
1	B	749	HIS
1	B	758	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

10 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	NAG	B	1227	1	14,14,15	0.63	0	17,19,21	1.01	1 (5%)
2	NAG	A	1227	1	14,14,15	0.64	0	17,19,21	1.00	1 (5%)
2	NAG	B	1083	1	14,14,15	1.10	1 (7%)	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1083	1	14,14,15	0.77	0	17,19,21	0.74	0
2	NAG	A	1319	1	14,14,15	0.65	0	17,19,21	1.45	1 (5%)
2	NAG	A	1521	1	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
2	NAG	B	1521	1	14,14,15	0.55	0	17,19,21	0.75	0
2	NAG	B	1090	1	14,14,15	0.84	1 (7%)	17,19,21	0.73	0
2	NAG	B	1319	1	14,14,15	0.74	0	17,19,21	1.66	3 (17%)
2	NAG	A	1090	1	14,14,15	1.29	2 (14%)	17,19,21	1.26	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1227	1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	A	1227	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	B	1083	1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	A	1090	1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	A	1319	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1521	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1521	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1090	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1319	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1083	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1083	NAG	C1-C2	3.26	1.57	1.52
2	A	1090	NAG	C1-C2	3.18	1.57	1.52
2	A	1090	NAG	C3-C2	2.99	1.58	1.52
2	B	1090	NAG	C1-C2	2.02	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1319	NAG	C4-C3-C2	-5.03	103.65	111.02
2	A	1319	NAG	C4-C3-C2	-4.33	104.67	111.02
2	A	1227	NAG	C4-C3-C2	-3.25	106.26	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1227	NAG	C4-C3-C2	-3.07	106.52	111.02
2	A	1090	NAG	C4-C3-C2	2.80	115.12	111.02
2	B	1319	NAG	C1-C2-N2	2.63	114.97	110.49
2	B	1319	NAG	O5-C1-C2	-2.26	107.71	111.29
2	A	1521	NAG	C4-C3-C2	-2.09	107.95	111.02

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1227	NAG	C1
2	A	1227	NAG	C1
2	B	1083	NAG	C1
2	A	1090	NAG	C1

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1227	NAG	C3-C2-N2-C7
2	A	1227	NAG	C3-C2-N2-C7
2	B	1083	NAG	C3-C2-N2-C7
2	A	1521	NAG	C3-C2-N2-C7
2	B	1521	NAG	C3-C2-N2-C7
2	B	1090	NAG	C3-C2-N2-C7
2	A	1090	NAG	C3-C2-N2-C7
2	A	1319	NAG	O5-C5-C6-O6
2	B	1521	NAG	O5-C5-C6-O6
2	B	1319	NAG	C1-C2-N2-C7
2	A	1319	NAG	C4-C5-C6-O6
2	B	1521	NAG	C4-C5-C6-O6
2	B	1227	NAG	O5-C5-C6-O6
2	B	1083	NAG	O5-C5-C6-O6
2	B	1227	NAG	C4-C5-C6-O6
2	B	1090	NAG	O5-C5-C6-O6
2	A	1083	NAG	O5-C5-C6-O6
2	A	1083	NAG	C3-C2-N2-C7
2	B	1083	NAG	C4-C5-C6-O6
2	A	1319	NAG	C1-C2-N2-C7
2	A	1090	NAG	C1-C2-N2-C7
2	B	1090	NAG	C4-C5-C6-O6
2	A	1090	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1227	NAG	4	0
2	A	1227	NAG	5	0
2	B	1083	NAG	2	0
2	A	1083	NAG	1	0
2	A	1521	NAG	2	0
2	B	1521	NAG	1	0
2	B	1090	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	730/730 (100%)	-0.28	11 (1%)	73	68	33, 54, 91, 147	0
1	B	730/730 (100%)	-0.13	18 (2%)	57	47	36, 63, 104, 161	0
All	All	1460/1460 (100%)	-0.20	29 (1%)	65	56	33, 58, 99, 161	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	ARG	6.3
1	B	442	ASN	4.9
1	B	393	GLN	4.6
1	B	392	GLU	4.5
1	A	392	GLU	3.9
1	A	391	PRO	3.8
1	B	376	LYS	3.0
1	A	94	GLU	2.9
1	B	438	THR	2.7
1	A	376	LYS	2.7
1	A	393	GLN	2.6
1	A	38	ARG	2.5
1	B	391	PRO	2.5
1	B	415	TYR	2.5
1	B	503	LYS	2.5
1	A	99	SER	2.4
1	B	348	ALA	2.3
1	B	401	GLY	2.3
1	B	444	LYS	2.2
1	A	98	ASP	2.2
1	A	522	GLU	2.2
1	B	138	ARG	2.2
1	B	469	TYR	2.2
1	B	439	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	217	ASN	2.2
1	B	124	HIS	2.1
1	A	52	ARG	2.1
1	B	464	LYS	2.0
1	B	157	GLN	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	1090	14/15	0.69	0.31	83,83,83,83	0
2	NAG	B	1083	14/15	0.70	0.34	108,108,108,108	0
2	NAG	A	1083	14/15	0.71	0.28	88,88,88,88	0
2	NAG	B	1521	14/15	0.74	0.40	102,102,102,102	0
2	NAG	B	1090	14/15	0.76	0.36	104,104,104,104	0
2	NAG	A	1521	14/15	0.76	0.33	110,110,110,110	0
2	NAG	B	1227	14/15	0.83	0.35	86,86,86,86	0
2	NAG	B	1319	14/15	0.85	0.30	68,68,68,68	0
2	NAG	A	1319	14/15	0.88	0.26	57,57,57,57	0
2	NAG	A	1227	14/15	0.90	0.31	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.