



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 04:36 PM EST

PDB ID : 1YSC  
Title : 2.8 ANGSTROMS STRUCTURE OF YEAST SERINE CARBOXYPEPTIDASE  
Authors : Endrizzi, J.A.; Remington, S.J.  
Deposited on : 1994-03-08  
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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

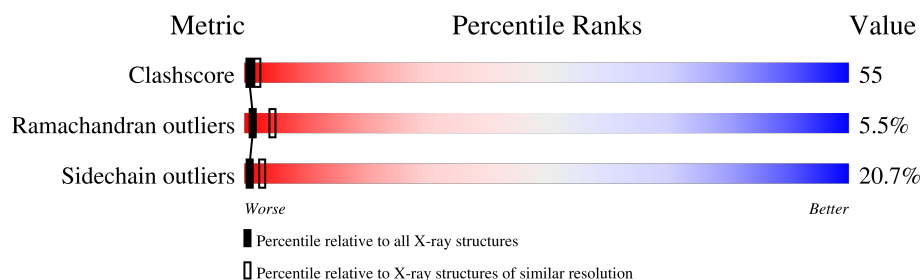
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	<div> <div></div> <div>28%</div> <div>50%</div> <div>19%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1681	X	-	-	-
2	NAG	A	3681	X	-	-	-
2	NAG	A	871	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3333 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 SERINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3253	2080	526	631	16			

- 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		

- Molecule 3 is water.

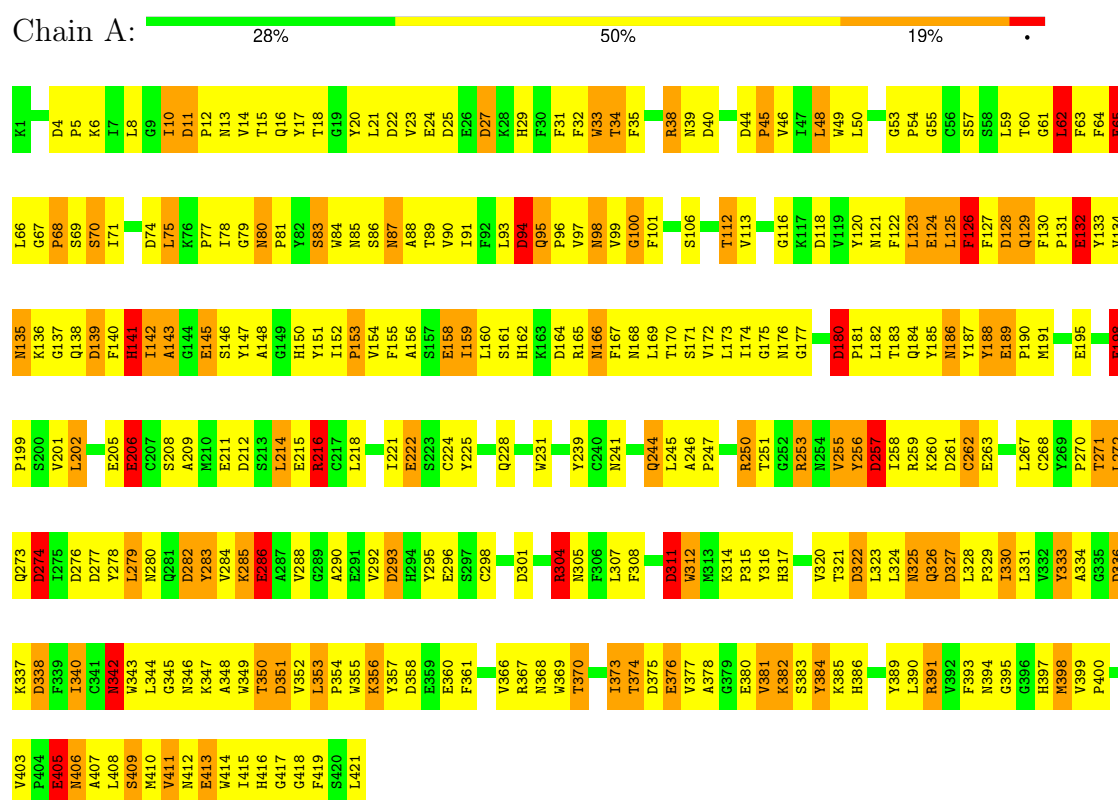
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0

### 3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

#### • Molecule 1: SERINE CARBOXYPEPTIDASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.80Å 111.80Å 111.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 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	1.15	21/3351 (0.6%)	1.65	67/4582 (1.5%)

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	4	0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLU	CD-OE2	9.35	1.35	1.25
1	A	189	GLU	CD-OE2	8.52	1.35	1.25
1	A	205	GLU	CD-OE1	7.64	1.34	1.25
1	A	380	GLU	CD-OE1	6.93	1.33	1.25
1	A	215	GLU	CD-OE2	6.82	1.33	1.25
1	A	222	GLU	CD-OE1	6.68	1.33	1.25
1	A	376	GLU	CD-OE1	6.67	1.32	1.25
1	A	286	GLU	CD-OE1	6.63	1.32	1.25
1	A	405	GLU	CD-OE2	6.38	1.32	1.25
1	A	360	GLU	CD-OE1	6.35	1.32	1.25
1	A	198	GLU	CD-OE2	6.33	1.32	1.25
1	A	211	GLU	CD-OE1	6.29	1.32	1.25
1	A	413	GLU	CD-OE1	6.20	1.32	1.25
1	A	263	GLU	CD-OE2	5.95	1.32	1.25
1	A	132	GLU	CD-OE2	5.86	1.32	1.25
1	A	206	GLU	CD-OE1	5.85	1.32	1.25
1	A	158	GLU	CD-OE2	5.79	1.32	1.25
1	A	195	GLU	CD-OE2	5.71	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLU	CD-OE1	5.50	1.31	1.25
1	A	124	GLU	CD-OE1	5.42	1.31	1.25
1	A	145	GLU	CD-OE1	5.32	1.31	1.25

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	A	322	ASP	CB-CG-OD1	8.43	125.89	118.30
1	A	74	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	A	293	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	A	322	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	25	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	A	257	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	A	367	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	A	293	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	188	TYR	CB-CG-CD1	-7.57	116.46	121.00
1	A	391	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	40	ASP	CB-CG-OD2	-7.51	111.55	118.30
1	A	336	ASP	CB-CG-OD2	7.35	124.92	118.30
1	A	301	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	A	327	ASP	CB-CG-OD1	7.18	124.77	118.30
1	A	74	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	164	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	A	94	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	338	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	311	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	261	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	274	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	A	164	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	212	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	375	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	143	ALA	CB-CA-C	6.62	120.04	110.10
1	A	336	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	A	312	TRP	N-CA-CB	-6.58	98.76	110.60
1	A	118	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	180	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	A	83	SER	N-CA-CB	6.44	120.16	110.50
1	A	27	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	384	TYR	N-CA-CB	6.33	121.99	110.60
1	A	253	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	11	ASP	CB-CG-OD2	6.16	123.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	212	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	153	PRO	N-CA-CB	6.03	110.54	103.30
1	A	325	ASN	CB-CA-C	6.02	122.45	110.40
1	A	25	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	27	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	A	216	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	40	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	48	LEU	CA-CB-CG	-5.83	101.90	115.30
1	A	126	PHE	CB-CG-CD1	5.82	124.88	120.80
1	A	188	TYR	CB-CG-CD2	5.79	124.48	121.00
1	A	342	ASN	CB-CA-C	-5.78	98.83	110.40
1	A	375	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	126	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	A	11	ASP	CB-CG-OD1	-5.73	113.15	118.30
1	A	304	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	353	LEU	C-N-CD	-5.53	108.44	120.60
1	A	256	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	A	22	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	180	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	128	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	80	ASN	CB-CA-C	5.32	121.05	110.40
1	A	282	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	367	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	334	ALA	CB-CA-C	-5.18	102.33	110.10
1	A	214	LEU	CB-CA-C	5.17	120.03	110.20
1	A	333	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	A	338	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	383	SER	N-CA-CB	5.06	118.08	110.50
1	A	125	LEU	CB-CA-C	-5.04	100.62	110.20
1	A	263	GLU	N-CA-CB	5.04	119.67	110.60
1	A	141	HIS	N-CA-CB	5.03	119.64	110.60

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	71	ILE	CA
1	A	275	ILE	CB
1	A	302	ILE	CB
1	A	415	ILE	CB

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	3253	0	2917	344	0
2	A	42	0	39	0	0
3	A	38	0	0	7	0
All	All	3333	0	2956	344	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 55.

All (344) 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:259:ARG:HD3	1:A:337:LYS:HD2	1.22	1.14
1:A:48:LEU:HB3	1:A:142:ILE:HG23	1.13	1.12
1:A:329:PRO:HA	1:A:386:HIS:HB2	1.37	1.07
1:A:38:ARG:HG3	1:A:86:SER:HA	1.29	1.05
1:A:173:LEU:HD23	1:A:331:LEU:HD22	1.42	0.99
1:A:143:ALA:HB2	1:A:173:LEU:HB2	1.46	0.95
1:A:5:PRO:HG3	1:A:18:THR:HG23	1.47	0.93
1:A:77:PRO:HD3	1:A:278:TYR:HE2	1.34	0.93
1:A:93:LEU:HD12	1:A:94:ASP:H	1.34	0.93
1:A:48:LEU:HD13	1:A:91:ILE:HB	1.52	0.88
1:A:328:LEU:HD23	1:A:329:PRO:HD2	1.55	0.87
1:A:77:PRO:HD3	1:A:278:TYR:CE2	2.09	0.87
1:A:259:ARG:HD3	1:A:337:LYS:CD	2.06	0.86
1:A:48:LEU:HB3	1:A:142:ILE:CG2	2.04	0.85
1:A:146:SER:HA	1:A:177:GLY:HA2	1.57	0.85
1:A:21:LEU:HD23	1:A:125:LEU:HB2	1.58	0.84
1:A:328:LEU:HD23	1:A:329:PRO:CD	2.07	0.84
1:A:355:TRP:CH2	1:A:357:TYR:HB2	2.13	0.84
1:A:57:SER:HB2	1:A:100:GLY:HA3	1.61	0.83
1:A:329:PRO:CA	1:A:386:HIS:HB2	2.10	0.82
1:A:202:LEU:HD23	1:A:206:GLU:HB3	1.61	0.81
1:A:191:MET:HG2	1:A:342:ASN:ND2	1.94	0.81
1:A:61:GLY:HA2	1:A:65:GLU:HG3	1.62	0.81
1:A:95:GLN:HG2	1:A:96:PRO:HA	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HG3	1:A:86:SER:CA	2.11	0.80
1:A:71:ILE:HD13	1:A:278:TYR:CG	2.15	0.80
1:A:214:LEU:HD11	1:A:218:LEU:HD11	1.63	0.79
1:A:20:TYR:HE2	1:A:290:ALA:HA	1.48	0.79
1:A:152:ILE:HD12	1:A:174:ILE:HG12	1.65	0.79
1:A:214:LEU:HD11	1:A:218:LEU:CD1	2.12	0.79
1:A:95:GLN:HG2	1:A:96:PRO:CA	2.14	0.79
1:A:171:SER:HA	1:A:328:LEU:HD21	1.65	0.78
1:A:133:TYR:O	1:A:138:GLN:HB2	1.84	0.78
1:A:352:VAL:O	1:A:354:PRO:HD3	1.84	0.77
1:A:369:TRP:CZ3	1:A:378:ALA:HB3	2.20	0.77
1:A:48:LEU:CB	1:A:142:ILE:HG23	2.06	0.77
1:A:61:GLY:HA2	1:A:65:GLU:CG	2.16	0.76
1:A:189:GLU:HB3	1:A:190:PRO:HD3	1.68	0.75
1:A:69:SER:HA	1:A:78:ILE:O	1.87	0.75
1:A:180:ASP:HB2	1:A:317:HIS:CG	2.21	0.75
1:A:84:TRP:CZ2	1:A:411:VAL:HG21	2.22	0.74
1:A:378:ALA:CB	1:A:406:ASN:HD22	1.99	0.74
1:A:283:TYR:O	1:A:286:GLU:HB2	1.87	0.74
1:A:180:ASP:OD2	1:A:183:THR:HB	1.87	0.74
1:A:180:ASP:HB2	1:A:317:HIS:CB	2.19	0.73
1:A:155:PHE:O	1:A:159:ILE:HG22	1.89	0.73
1:A:10:ILE:HG23	1:A:69:SER:CB	2.19	0.72
1:A:201:VAL:HG23	1:A:202:LEU:HD12	1.69	0.72
1:A:180:ASP:HB2	1:A:317:HIS:HB3	1.71	0.72
1:A:411:VAL:O	1:A:415:ILE:HG23	1.90	0.71
1:A:398:MET:HG3	3:A:486:HOH:O	1.90	0.71
1:A:123:LEU:HB3	1:A:167:PHE:CZ	2.25	0.71
1:A:408:LEU:HD11	1:A:412:ASN:ND2	2.05	0.71
1:A:408:LEU:HD12	1:A:408:LEU:O	1.91	0.71
1:A:173:LEU:CD2	1:A:331:LEU:HD22	2.20	0.71
1:A:320:VAL:HG12	1:A:353:LEU:HD21	1.73	0.71
1:A:355:TRP:O	1:A:358:ASP:HB2	1.91	0.71
1:A:93:LEU:HD12	1:A:94:ASP:N	2.05	0.70
1:A:21:LEU:HD21	1:A:126:PHE:CA	2.21	0.70
1:A:191:MET:HG2	1:A:342:ASN:HD21	1.55	0.70
1:A:48:LEU:HD12	1:A:49:TRP:N	2.06	0.70
1:A:181:PRO:HD2	1:A:225:TYR:OH	1.92	0.70
1:A:146:SER:CA	1:A:177:GLY:HA2	2.22	0.69
1:A:331:LEU:HD23	1:A:331:LEU:O	1.91	0.69
1:A:21:LEU:HD21	1:A:126:PHE:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:HA	1:A:337:LYS:O	1.93	0.68
1:A:355:TRP:CZ2	1:A:357:TYR:HB2	2.29	0.68
1:A:65:GLU:O	1:A:400:PRO:HB2	1.94	0.68
1:A:125:LEU:N	1:A:125:LEU:HD23	2.06	0.68
1:A:18:THR:HG21	1:A:33:TRP:CD2	2.28	0.67
1:A:336:ASP:OD1	1:A:394:ASN:N	2.27	0.67
1:A:121:ASN:O	1:A:125:LEU:HG	1.95	0.67
1:A:57:SER:HB2	1:A:100:GLY:CA	2.23	0.67
1:A:5:PRO:HG3	1:A:18:THR:CG2	2.20	0.66
1:A:8:LEU:HD21	1:A:284:VAL:HA	1.77	0.66
1:A:214:LEU:CD1	1:A:218:LEU:HG	2.24	0.66
1:A:218:LEU:HD23	1:A:221:ILE:HD12	1.77	0.66
1:A:327:ASP:OD1	1:A:356:LYS:NZ	2.28	0.66
1:A:112:THR:HG22	1:A:113:VAL:N	2.10	0.65
1:A:280:ASN:O	1:A:285:LYS:HE3	1.96	0.65
1:A:304:ARG:NH1	1:A:305:ASN:OD1	2.30	0.65
1:A:373:ILE:HG22	1:A:374:THR:N	2.10	0.65
1:A:95:GLN:CG	1:A:96:PRO:HA	2.26	0.65
1:A:206:GLU:OE1	1:A:247:PRO:HB3	1.97	0.65
1:A:53:GLY:HA3	1:A:54:PRO:C	2.17	0.64
1:A:337:LYS:N	1:A:395:GLY:O	2.28	0.64
1:A:27:ASP:OD1	1:A:29:HIS:NE2	2.28	0.64
1:A:126:PHE:HE1	1:A:127:PHE:CE1	2.16	0.64
1:A:329:PRO:HA	1:A:386:HIS:O	1.97	0.64
1:A:141:HIS:HB3	1:A:171:SER:O	1.97	0.64
1:A:183:THR:O	1:A:186:ASN:ND2	2.32	0.63
1:A:67:GLY:O	1:A:83:SER:HB2	1.99	0.63
1:A:71:ILE:HD13	1:A:278:TYR:CD2	2.33	0.63
1:A:71:ILE:HD13	1:A:278:TYR:CB	2.28	0.63
1:A:143:ALA:CB	1:A:173:LEU:HB2	2.27	0.62
1:A:378:ALA:HB1	1:A:406:ASN:HD22	1.64	0.62
1:A:133:TYR:HA	1:A:138:GLN:NE2	2.14	0.62
1:A:378:ALA:HB2	1:A:406:ASN:HD22	1.63	0.62
1:A:20:TYR:CE1	1:A:31:PHE:HB2	2.33	0.62
1:A:134:VAL:O	1:A:137:GLY:N	2.32	0.62
1:A:159:ILE:HD13	1:A:169:LEU:HD22	1.82	0.62
1:A:172:VAL:HG23	1:A:330:ILE:HG23	1.81	0.62
1:A:274:ASP:O	1:A:277:ASP:HB2	1.99	0.61
1:A:5:PRO:CG	1:A:18:THR:HG23	2.26	0.61
1:A:131:PRO:HD2	1:A:132:GLU:CG	2.30	0.61
1:A:328:LEU:HD23	1:A:329:PRO:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:MET:CE	1:A:411:VAL:HG23	2.31	0.61
1:A:136:LYS:HB2	1:A:138:GLN:OE1	2.01	0.61
1:A:5:PRO:HG2	1:A:16:GLN:CB	2.31	0.61
1:A:150:HIS:O	1:A:154:VAL:HG23	2.02	0.60
1:A:271:THR:HA	1:A:274:ASP:OD2	2.01	0.60
1:A:214:LEU:HD12	1:A:218:LEU:HG	1.82	0.60
1:A:324:LEU:HD12	1:A:353:LEU:HD21	1.81	0.60
1:A:48:LEU:CD1	1:A:91:ILE:HB	2.30	0.60
1:A:31:PHE:HE2	1:A:288:VAL:CG1	2.15	0.59
1:A:406:ASN:HA	1:A:409:SER:HB2	1.85	0.59
1:A:45:PRO:HG2	1:A:415:ILE:CG1	2.33	0.59
1:A:188:TYR:HB2	1:A:244:GLN:HG2	1.85	0.59
1:A:361:PHE:CE1	1:A:382:LYS:HD2	2.37	0.59
1:A:328:LEU:CD2	1:A:329:PRO:HD2	2.31	0.58
1:A:378:ALA:O	1:A:393:PHE:HB2	2.03	0.58
1:A:145:GLU:HA	1:A:175:GLY:O	2.03	0.58
1:A:60:THR:O	1:A:64:PHE:HB3	2.02	0.58
1:A:130:PHE:HA	1:A:132:GLU:OE2	2.04	0.58
1:A:189:GLU:HB3	1:A:190:PRO:CD	2.33	0.58
1:A:273:GLN:NE2	1:A:273:GLN:HA	2.19	0.58
1:A:381:VAL:HG13	1:A:390:LEU:HD13	1.86	0.57
1:A:413:GLU:HG2	1:A:421:LEU:CD2	2.35	0.56
1:A:206:GLU:O	1:A:209:ALA:HB3	2.04	0.56
1:A:20:TYR:CE2	1:A:290:ALA:HA	2.35	0.56
1:A:198:GLU:HG3	1:A:199:PRO:HD2	1.87	0.56
1:A:61:GLY:CA	1:A:65:GLU:HG3	2.35	0.56
1:A:96:PRO:N	1:A:99:VAL:HG21	2.21	0.56
1:A:77:PRO:O	1:A:78:ILE:HG13	2.06	0.56
1:A:160:LEU:HD12	1:A:323:LEU:HD23	1.88	0.56
1:A:59:LEU:O	1:A:62:LEU:HB3	2.06	0.56
1:A:96:PRO:O	1:A:99:VAL:HB	2.06	0.56
1:A:48:LEU:HD12	1:A:49:TRP:H	1.69	0.55
1:A:127:PHE:HD2	1:A:167:PHE:CD1	2.24	0.55
1:A:147:TYR:O	1:A:150:HIS:HB2	2.06	0.55
1:A:131:PRO:HD2	1:A:132:GLU:HG3	1.89	0.55
1:A:95:GLN:HG2	1:A:96:PRO:N	2.20	0.55
1:A:176:ASN:HB2	3:A:458:HOH:O	2.06	0.55
1:A:185:TYR:OH	1:A:241:ASN:ND2	2.40	0.55
1:A:38:ARG:HD3	1:A:85:ASN:HD21	1.71	0.55
1:A:83:SER:O	1:A:408:LEU:HD22	2.06	0.55
1:A:70:SER:C	1:A:71:ILE:HG13	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:SER:HA	1:A:328:LEU:CD2	2.36	0.54
1:A:34:THR:HG22	1:A:35:PHE:H	1.73	0.54
1:A:282:ASP:O	1:A:286:GLU:HG2	2.08	0.54
1:A:357:TYR:HB3	1:A:384:TYR:CE1	2.41	0.54
1:A:410:MET:HE3	1:A:411:VAL:HG23	1.90	0.54
1:A:62:LEU:HD13	1:A:63:PHE:CE2	2.43	0.54
1:A:159:ILE:HG23	1:A:160:LEU:H	1.72	0.54
1:A:64:PHE:CZ	1:A:272:LEU:HD21	2.43	0.54
1:A:330:ILE:N	1:A:386:HIS:O	2.37	0.53
1:A:95:GLN:HG3	3:A:476:HOH:O	2.08	0.53
1:A:366:VAL:HA	1:A:381:VAL:O	2.08	0.53
1:A:317:HIS:H	1:A:317:HIS:CD2	2.26	0.53
1:A:183:THR:HG21	1:A:349:TRP:HA	1.90	0.53
1:A:46:VAL:HG21	1:A:133:TYR:HB3	1.90	0.53
1:A:214:LEU:HD11	1:A:218:LEU:HG	1.90	0.53
1:A:416:HIS:O	1:A:418:GLY:N	2.35	0.53
1:A:324:LEU:HD12	1:A:353:LEU:CD2	2.38	0.52
1:A:407:ALA:O	1:A:411:VAL:N	2.36	0.52
1:A:130:PHE:HB3	1:A:133:TYR:CE2	2.44	0.52
1:A:64:PHE:CE1	1:A:272:LEU:HD23	2.44	0.52
1:A:130:PHE:C	1:A:132:GLU:HG3	2.30	0.52
1:A:411:VAL:HG12	1:A:412:ASN:HD22	1.75	0.52
1:A:23:VAL:O	1:A:23:VAL:HG13	2.09	0.52
1:A:382:LYS:HB2	3:A:469:HOH:O	2.09	0.52
1:A:127:PHE:HD2	1:A:167:PHE:CG	2.27	0.52
1:A:214:LEU:HD11	1:A:218:LEU:CG	2.40	0.52
1:A:127:PHE:CD2	1:A:167:PHE:CG	2.97	0.51
1:A:198:GLU:OE2	1:A:259:ARG:HG2	2.10	0.51
1:A:5:PRO:HB3	1:A:33:TRP:CZ2	2.45	0.51
1:A:89:THR:HG22	3:A:461:HOH:O	2.09	0.51
1:A:270:PRO:HD2	3:A:484:HOH:O	2.10	0.51
1:A:155:PHE:CD1	1:A:155:PHE:N	2.77	0.51
1:A:349:TRP:HZ3	1:A:353:LEU:HD13	1.75	0.51
1:A:180:ASP:CB	1:A:317:HIS:HB3	2.39	0.51
1:A:61:GLY:HA2	1:A:65:GLU:OE2	2.10	0.51
1:A:406:ASN:N	1:A:406:ASN:OD1	2.42	0.51
1:A:384:TYR:CE1	1:A:385:LYS:HG3	2.46	0.51
1:A:66:LEU:HD23	1:A:400:PRO:HG2	1.92	0.51
1:A:214:LEU:HD12	1:A:214:LEU:O	2.10	0.51
1:A:378:ALA:HB2	1:A:406:ASN:ND2	2.25	0.51
1:A:10:ILE:HG22	1:A:11:ASP:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:CD1	1:A:323:LEU:HD23	2.40	0.50
1:A:140:PHE:CD1	1:A:141:HIS:N	2.80	0.50
1:A:8:LEU:HB3	1:A:10:ILE:HD12	1.92	0.50
1:A:18:THR:HG22	1:A:33:TRP:HA	1.92	0.50
1:A:152:ILE:HD12	1:A:174:ILE:CG1	2.39	0.50
1:A:198:GLU:HG3	1:A:199:PRO:CD	2.42	0.50
1:A:216:ARG:HG2	1:A:239:TYR:CZ	2.46	0.50
1:A:84:TRP:CH2	1:A:411:VAL:HG21	2.46	0.49
1:A:160:LEU:HD12	1:A:323:LEU:CD2	2.42	0.49
1:A:338:ASP:OD1	1:A:340:ILE:HG22	2.12	0.49
1:A:29:HIS:CD2	1:A:29:HIS:N	2.79	0.49
1:A:34:THR:HG22	1:A:35:PHE:N	2.27	0.49
1:A:45:PRO:HB3	1:A:139:ASP:O	2.12	0.49
1:A:148:ALA:HA	1:A:151:TYR:HB2	1.95	0.49
1:A:406:ASN:O	1:A:409:SER:HB2	2.12	0.49
1:A:94:ASP:OD2	1:A:101:PHE:N	2.36	0.49
1:A:283:TYR:HD1	1:A:283:TYR:H	1.58	0.49
1:A:71:ILE:CG2	1:A:75:LEU:HD12	2.42	0.49
1:A:391:ARG:O	1:A:391:ARG:HG2	2.11	0.49
1:A:4:ASP:C	1:A:6:LYS:H	2.15	0.49
1:A:141:HIS:N	1:A:141:HIS:CD2	2.79	0.49
1:A:94:ASP:OD2	1:A:100:GLY:HA3	2.13	0.49
1:A:180:ASP:OD2	1:A:349:TRP:HB2	2.13	0.49
1:A:32:PHE:CD1	1:A:32:PHE:N	2.79	0.48
1:A:166:ASN:OD1	1:A:167:PHE:HD1	1.96	0.48
1:A:126:PHE:CE1	1:A:127:PHE:CE1	2.98	0.48
1:A:158:GLU:OE1	1:A:158:GLU:HA	2.12	0.48
1:A:180:ASP:O	1:A:184:GLN:HG3	2.12	0.48
1:A:125:LEU:O	1:A:129:GLN:HG2	2.14	0.48
1:A:80:ASN:ND2	1:A:83:SER:HA	2.28	0.48
1:A:320:VAL:HG12	1:A:353:LEU:CD2	2.43	0.48
1:A:64:PHE:CD1	1:A:272:LEU:HD23	2.49	0.48
1:A:100:GLY:HA2	1:A:295:TYR:CE2	2.49	0.48
1:A:270:PRO:O	1:A:273:GLN:N	2.39	0.48
1:A:354:PRO:O	1:A:355:TRP:HB3	2.13	0.48
1:A:181:PRO:O	1:A:185:TYR:HB2	2.13	0.47
1:A:148:ALA:HA	1:A:151:TYR:CD2	2.48	0.47
1:A:71:ILE:CD1	1:A:278:TYR:CG	2.93	0.47
1:A:409:SER:O	1:A:413:GLU:HB3	2.14	0.47
1:A:18:THR:HG21	1:A:33:TRP:CG	2.48	0.47
1:A:77:PRO:HG3	1:A:278:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:THR:HG22	1:A:351:ASP:N	2.29	0.47
1:A:131:PRO:CD	1:A:132:GLU:HG3	2.44	0.47
1:A:140:PHE:HB3	1:A:168:ASN:O	2.14	0.47
1:A:307:LEU:HD23	1:A:308:PHE:CE2	2.48	0.47
1:A:79:GLY:O	1:A:81:PRO:HD3	2.15	0.47
1:A:142:ILE:HD11	1:A:169:LEU:HD13	1.96	0.47
1:A:146:SER:HA	1:A:176:ASN:O	2.14	0.47
1:A:247:PRO:HA	1:A:250:ARG:HG3	1.97	0.47
1:A:62:LEU:HD23	1:A:67:GLY:HA3	1.96	0.47
1:A:97:VAL:HG12	1:A:98:ASN:ND2	2.28	0.47
1:A:331:LEU:HD23	1:A:331:LEU:C	2.35	0.47
1:A:180:ASP:N	1:A:184:GLN:OE1	2.38	0.47
1:A:46:VAL:HG22	1:A:89:THR:CG2	2.46	0.46
1:A:44:ASP:HB3	1:A:88:ALA:HA	1.96	0.46
1:A:96:PRO:CD	1:A:99:VAL:HG21	2.45	0.46
1:A:68:PRO:O	1:A:80:ASN:N	2.48	0.46
1:A:152:ILE:HB	1:A:153:PRO:HD3	1.97	0.46
1:A:256:TYR:O	1:A:257:ASP:HB2	2.14	0.46
1:A:112:THR:HG22	1:A:154:VAL:HG11	1.97	0.46
1:A:39:ASN:HB3	1:A:44:ASP:OD2	2.16	0.46
1:A:100:GLY:CA	1:A:295:TYR:CE2	2.99	0.46
1:A:182:LEU:HB2	1:A:225:TYR:CE2	2.51	0.46
1:A:5:PRO:HD2	1:A:17:TYR:HA	1.97	0.46
1:A:172:VAL:CG2	1:A:330:ILE:HD13	2.45	0.46
1:A:21:LEU:HD21	1:A:126:PHE:N	2.29	0.46
1:A:201:VAL:HG23	1:A:202:LEU:CD1	2.42	0.46
1:A:34:THR:HG23	1:A:90:VAL:O	2.16	0.46
1:A:222:GLU:O	1:A:225:TYR:HB2	2.16	0.46
1:A:384:TYR:CE1	1:A:385:LYS:CG	2.99	0.46
1:A:116:GLY:HA3	1:A:155:PHE:CD1	2.51	0.45
1:A:133:TYR:HA	1:A:138:GLN:HE22	1.79	0.45
1:A:172:VAL:HG21	1:A:330:ILE:HD13	1.97	0.45
1:A:202:LEU:HD21	1:A:247:PRO:HB2	1.98	0.45
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.56	0.45
1:A:322:ASP:O	1:A:326:GLN:HG3	2.15	0.45
1:A:343:TRP:CZ2	1:A:344:LEU:CD2	2.99	0.45
1:A:346:ASN:HA	1:A:349:TRP:CD1	2.51	0.45
1:A:64:PHE:CE1	1:A:272:LEU:CD2	3.00	0.45
1:A:390:LEU:HD22	1:A:421:LEU:HD13	1.99	0.45
1:A:21:LEU:CD2	1:A:125:LEU:HB2	2.39	0.45
1:A:198:GLU:HA	1:A:199:PRO:HD3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:THR:HG23	1:A:354:PRO:O	2.17	0.45
1:A:279:LEU:HD12	1:A:279:LEU:HA	1.80	0.45
1:A:182:LEU:CB	1:A:225:TYR:CE2	3.00	0.45
1:A:412:ASN:HD22	1:A:412:ASN:N	2.14	0.45
1:A:390:LEU:HD22	1:A:421:LEU:CD1	2.46	0.45
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.17	0.45
1:A:399:VAL:N	1:A:400:PRO:CD	2.79	0.45
1:A:96:PRO:HD2	1:A:99:VAL:HG21	1.98	0.44
1:A:159:ILE:HD11	1:A:169:LEU:HB2	1.99	0.44
1:A:273:GLN:HA	1:A:273:GLN:HE21	1.82	0.44
1:A:132:GLU:HG3	1:A:132:GLU:H	0.90	0.44
1:A:120:TYR:CD2	1:A:159:ILE:HA	2.53	0.44
1:A:202:LEU:HD23	1:A:206:GLU:CB	2.40	0.44
1:A:187:TYR:CD2	1:A:345:GLY:HA2	2.52	0.44
1:A:50:LEU:N	1:A:143:ALA:O	2.50	0.44
1:A:262:CYS:HB2	1:A:268:CYS:HA	2.00	0.44
1:A:116:GLY:CA	1:A:155:PHE:CD1	3.00	0.43
1:A:191:MET:HE3	1:A:338:ASP:O	2.18	0.43
1:A:127:PHE:HD1	1:A:127:PHE:HA	1.55	0.43
1:A:411:VAL:C	1:A:415:ILE:HG23	2.37	0.43
1:A:112:THR:CG2	1:A:154:VAL:HG11	2.48	0.43
1:A:273:GLN:NE2	1:A:273:GLN:CA	2.81	0.43
1:A:370:THR:O	1:A:370:THR:HG22	2.17	0.43
1:A:55:GLY:O	1:A:298:CYS:HA	2.17	0.43
1:A:246:ALA:O	1:A:250:ARG:HG2	2.19	0.43
1:A:173:LEU:HD11	1:A:414:TRP:CD1	2.54	0.43
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.56	0.43
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.89	0.43
1:A:84:TRP:CZ2	1:A:411:VAL:CG2	2.97	0.42
1:A:131:PRO:N	1:A:132:GLU:HG3	2.34	0.42
1:A:112:THR:HG21	1:A:154:VAL:HG21	2.01	0.42
1:A:146:SER:O	1:A:177:GLY:HA2	2.18	0.42
1:A:255:VAL:HG13	1:A:340:ILE:HB	2.01	0.42
1:A:405:GLU:H	1:A:405:GLU:HG2	1.44	0.42
1:A:126:PHE:CE1	1:A:127:PHE:CD1	3.07	0.42
1:A:350:THR:HG21	1:A:389:TYR:HB2	2.00	0.42
1:A:87:ASN:HB2	1:A:412:ASN:OD1	2.20	0.42
1:A:153:PRO:O	1:A:156:ALA:HB3	2.20	0.42
1:A:331:LEU:CD2	1:A:333:TYR:HD1	2.33	0.42
1:A:343:TRP:CZ2	1:A:344:LEU:HD23	2.54	0.42
1:A:347:LYS:O	1:A:350:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HG12	1:A:412:ASN:N	2.33	0.42
1:A:130:PHE:C	1:A:132:GLU:H	2.23	0.42
1:A:386:HIS:CD2	1:A:386:HIS:H	2.37	0.42
1:A:273:GLN:HE21	1:A:273:GLN:CA	2.33	0.42
1:A:317:HIS:O	1:A:320:VAL:HB	2.20	0.42
1:A:38:ARG:HG2	1:A:85:ASN:O	2.20	0.42
1:A:143:ALA:HA	1:A:173:LEU:O	2.19	0.42
1:A:241:ASN:ND2	1:A:245:LEU:HD11	2.34	0.42
1:A:123:LEU:HD11	1:A:140:PHE:CZ	2.55	0.41
1:A:83:SER:OG	1:A:85:ASN:OD1	2.38	0.41
1:A:186:ASN:ND2	1:A:186:ASN:H	2.18	0.41
1:A:4:ASP:C	1:A:6:LYS:N	2.73	0.41
1:A:18:THR:CG2	1:A:33:TRP:CD2	3.00	0.41
1:A:216:ARG:HA	3:A:485:HOH:O	2.19	0.41
1:A:256:TYR:HB3	1:A:397:HIS:HB3	2.02	0.41
1:A:331:LEU:HD21	1:A:333:TYR:CD1	2.56	0.41
1:A:131:PRO:HD2	1:A:132:GLU:HG2	2.02	0.41
1:A:317:HIS:CD2	1:A:317:HIS:N	2.88	0.41
1:A:348:ALA:HA	1:A:351:ASP:HB2	2.02	0.41
1:A:31:PHE:CE2	1:A:288:VAL:CG1	2.99	0.41
1:A:369:TRP:CE3	1:A:378:ALA:HB3	2.55	0.41
1:A:154:VAL:CG2	1:A:316:TYR:CD1	3.03	0.41
1:A:162:HIS:ND1	1:A:162:HIS:N	2.68	0.41
1:A:384:TYR:CE1	1:A:385:LYS:HE3	2.55	0.41
1:A:159:ILE:HG23	1:A:160:LEU:N	2.34	0.41
1:A:325:ASN:OD1	1:A:356:LYS:HD2	2.21	0.41
1:A:106:SER:O	1:A:106:SER:OG	2.33	0.40
1:A:95:GLN:HA	1:A:96:PRO:C	2.41	0.40
1:A:189:GLU:N	1:A:190:PRO:HD2	2.36	0.40
1:A:224:CYS:O	1:A:228:GLN:N	2.54	0.40
1:A:315:PRO:HA	1:A:317:HIS:HD2	1.86	0.40
1:A:403:VAL:O	1:A:403:VAL:HG23	2.22	0.40
1:A:31:PHE:CD1	1:A:31:PHE:C	2.94	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	419/421 (100%)	340 (81%)	56 (13%)	23 (6%)	<b>1</b> <b>4</b>

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	13	ASN
1	A	15	THR
1	A	24	GLU
1	A	135	ASN
1	A	417	GLY
1	A	419	PHE
1	A	10	ILE
1	A	231	TRP
1	A	311	ASP
1	A	342	ASN
1	A	100	GLY
1	A	165	ARG
1	A	312	TRP
1	A	98	ASN
1	A	411	VAL
1	A	14	VAL
1	A	62	LEU
1	A	257	ASP
1	A	271	THR
1	A	373	ILE
1	A	45	PRO
1	A	68	PRO

### 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	334/365 (92%)	265 (79%)	69 (21%)	<b>1</b> <b>3</b>

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TRP
1	A	34	THR
1	A	38	ARG
1	A	62	LEU
1	A	65	GLU
1	A	70	SER
1	A	75	LEU
1	A	87	ASN
1	A	94	ASP
1	A	95	GLN
1	A	112	THR
1	A	122	PHE
1	A	123	LEU
1	A	124	GLU
1	A	126	PHE
1	A	128	ASP
1	A	129	GLN
1	A	132	GLU
1	A	135	ASN
1	A	139	ASP
1	A	141	HIS
1	A	142	ILE
1	A	159	ILE
1	A	161	SER
1	A	166	ASN
1	A	170	THR
1	A	180	ASP
1	A	186	ASN
1	A	198	GLU
1	A	202	LEU

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Mol	Chain	Res	Type
1	A	206	GLU
1	A	208	SER
1	A	216	ARG
1	A	244	GLN
1	A	250	ARG
1	A	251	THR
1	A	253	ARG
1	A	255	VAL
1	A	258	ILE
1	A	260	LYS
1	A	262	CYS
1	A	272	LEU
1	A	274	ASP
1	A	276	ASP
1	A	279	LEU
1	A	283	TYR
1	A	285	LYS
1	A	286	GLU
1	A	292	VAL
1	A	293	ASP
1	A	304	ARG
1	A	311	ASP
1	A	314	LYS
1	A	326	GLN
1	A	330	ILE
1	A	340	ILE
1	A	350	THR
1	A	356	LYS
1	A	368	ASN
1	A	370	THR
1	A	374	THR
1	A	376	GLU
1	A	377	VAL
1	A	381	VAL
1	A	382	LYS
1	A	398	MET
1	A	405	GLU
1	A	406	ASN
1	A	409	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	129	GLN
1	A	241	ASN
1	A	244	GLN
1	A	273	GLN
1	A	303	ASN
1	A	317	HIS
1	A	342	ASN
1	A	386	HIS
1	A	412	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	A	1681	1	14,14,15	1.40	3 (21%)	17,19,21	2.23	4 (23%)
2	NAG	A	871	1	14,14,15	1.29	2 (14%)	17,19,21	4.09	5 (29%)
2	NAG	A	3681	1	14,14,15	0.68	0	17,19,21	1.47	3 (17%)

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	A	1681	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	871	1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	A	3681	1	1/1/5/7	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	871	NAG	C1-C2	3.39	1.57	1.52
2	A	1681	NAG	C1-C2	2.84	1.56	1.52
2	A	1681	NAG	C2-N2	2.52	1.50	1.46
2	A	871	NAG	C2-N2	2.24	1.50	1.46
2	A	1681	NAG	C3-C2	2.03	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	871	NAG	O6-C6-C5	13.02	155.68	111.33
2	A	871	NAG	C1-O5-C5	7.52	122.27	112.19
2	A	1681	NAG	O6-C6-C5	5.61	130.45	111.33
2	A	1681	NAG	C2-N2-C7	4.38	128.77	122.90
2	A	1681	NAG	O7-C7-C8	-4.33	114.34	122.05
2	A	871	NAG	O5-C1-C2	4.25	117.86	111.29
2	A	871	NAG	C1-C2-N2	3.67	116.22	110.43
2	A	3681	NAG	O6-C6-C5	3.62	123.67	111.33
2	A	871	NAG	O7-C7-C8	-3.25	116.26	122.05
2	A	3681	NAG	C3-C4-C5	2.67	115.07	110.23
2	A	3681	NAG	C4-C3-C2	2.10	114.09	111.02
2	A	1681	NAG	O7-C7-N2	2.01	125.54	121.98

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	871	NAG	C1
2	A	1681	NAG	C1
2	A	3681	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	871	NAG	C3-C2-N2-C7
2	A	1681	NAG	C8-C7-N2-C2
2	A	1681	NAG	O7-C7-N2-C2
2	A	3681	NAG	C8-C7-N2-C2
2	A	3681	NAG	O7-C7-N2-C2
2	A	3681	NAG	O5-C5-C6-O6
2	A	1681	NAG	O5-C5-C6-O6
2	A	1681	NAG	C4-C5-C6-O6
2	A	871	NAG	C8-C7-N2-C2
2	A	871	NAG	O7-C7-N2-C2
2	A	3681	NAG	C4-C5-C6-O6

There are no ring outliers.

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 [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.