



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 09:43 AM BST

PDB ID : 1CPY
Title : SITE-DIRECTED MUTAGENESIS ON (SERINE) CARBOXYPEPTIDASE
Y FROM YEAST. THE SIGNIFICANCE OF THR 60 AND MET 398 IN
HYDROLYSIS AND AMINOLYSIS REACTIONS
Authors : Sorensen, S.B.; Raaschou-Nielsen, M.; Mortensen, U.; Remington, S.J.; Bred-
dam, K.
Deposited on : 1995-03-24
Resolution : 2.60 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

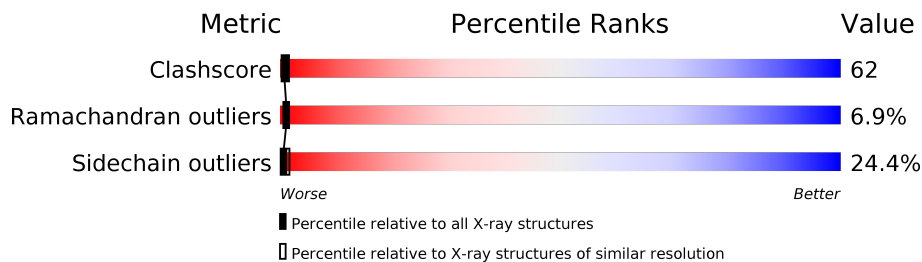
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3325 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.

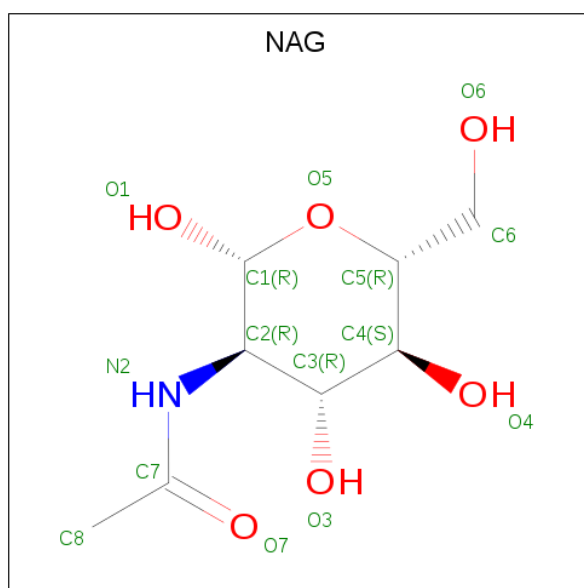
- Molecule 1 is a protein called SERINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3245	2076	526	627	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ALA	GLU	conflict	UNP P00729
A	145	ALA	GLU	conflict	UNP P00729

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

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

- Molecule 3 is water.

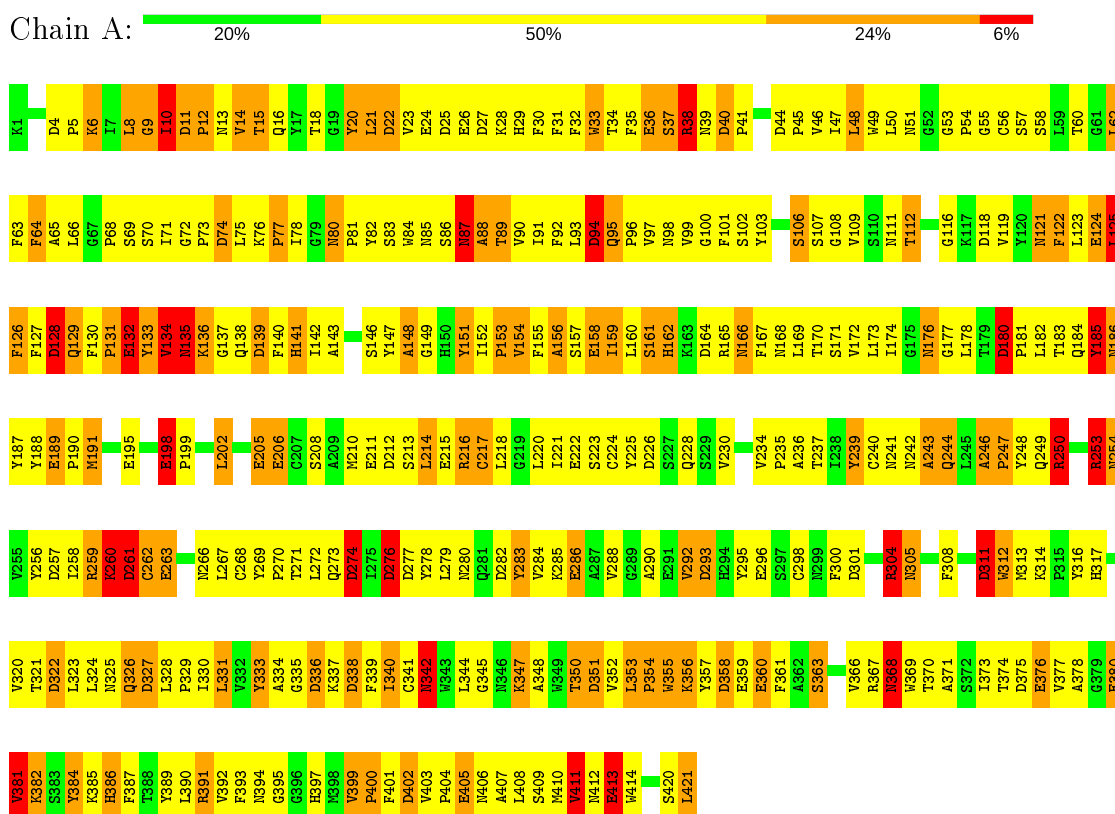
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		

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

Xtrriage (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, α , β , γ	112.00Å 112.00Å 112.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3325	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.99	26/3343 (0.8%)	1.91	103/4572 (2.3%)

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

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	LEU	C-OXT	79.24	2.73	1.23
1	A	222	GLU	CD-OE1	10.92	1.37	1.25
1	A	205	GLU	CD-OE1	10.38	1.37	1.25
1	A	263	GLU	CD-OE2	9.05	1.35	1.25
1	A	405	GLU	CD-OE2	9.03	1.35	1.25
1	A	198	GLU	CD-OE2	7.01	1.33	1.25
1	A	413	GLU	CD-OE1	6.99	1.33	1.25
1	A	376	GLU	CD-OE2	6.94	1.33	1.25
1	A	215	GLU	CD-OE1	6.88	1.33	1.25
1	A	211	GLU	CD-OE1	6.74	1.33	1.25
1	A	286	GLU	CD-OE1	6.70	1.33	1.25
1	A	189	GLU	CD-OE2	6.62	1.32	1.25
1	A	158	GLU	CD-OE2	6.46	1.32	1.25
1	A	360	GLU	CD-OE1	6.29	1.32	1.25
1	A	206	GLU	CD-OE2	6.14	1.32	1.25
1	A	195	GLU	CD-OE2	6.06	1.32	1.25
1	A	124	GLU	CD-OE1	5.88	1.32	1.25
1	A	380	GLU	CD-OE2	-5.67	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	GLU	CD-OE2	5.52	1.31	1.25
1	A	132	GLU	CD-OE1	-5.49	1.19	1.25
1	A	367	ARG	NE-CZ	5.48	1.40	1.33
1	A	333	TYR	CA-CB	-5.44	1.42	1.53
1	A	296	GLU	CD-OE1	5.42	1.31	1.25
1	A	36	GLU	CD-OE1	5.12	1.31	1.25
1	A	400	PRO	CA-C	-5.10	1.42	1.52
1	A	250	ARG	NE-CZ	5.07	1.39	1.33

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	LEU	C-N-CD	-13.50	90.91	120.60
1	A	391	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	A	40	ASP	CB-CG-OD2	-10.74	108.64	118.30
1	A	304	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	367	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	A	25	ASP	CB-CG-OD2	-9.02	110.18	118.30
1	A	338	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	A	259	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	A	293	ASP	CB-CG-OD1	8.24	125.72	118.30
1	A	293	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	A	301	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	A	74	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	276	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	304	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	40	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	375	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	327	ASP	CB-CG-OD1	7.46	125.02	118.30
1	A	411	VAL	CA-CB-CG2	-7.39	99.82	110.90
1	A	259	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	322	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	347	LYS	CB-CA-C	-7.29	95.81	110.40
1	A	237	THR	CA-CB-CG2	-7.25	102.24	112.40
1	A	261	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	A	311	ASP	CB-CG-OD2	6.98	124.58	118.30
1	A	243	ALA	CB-CA-C	-6.97	99.65	110.10
1	A	180	ASP	CB-CG-OD2	6.93	124.53	118.30
1	A	21	LEU	CB-CG-CD1	-6.91	99.25	111.00
1	A	87	ASN	N-CA-CB	-6.90	98.18	110.60
1	A	322	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	247	PRO	N-CA-CB	6.85	111.52	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	259	ARG	CD-NE-CZ	6.81	133.14	123.60
1	A	381	VAL	CA-CB-CG2	6.76	121.03	110.90
1	A	368	ASN	N-CA-CB	6.72	122.69	110.60
1	A	74	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	151	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	A	94	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	311	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	A	342	ASN	CB-CA-C	-6.35	97.71	110.40
1	A	274	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	A	25	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	250	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	A	27	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	333	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	A	22	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	A	280	ASN	CB-CA-C	-6.11	98.18	110.40
1	A	312	TRP	CB-CA-C	-6.10	98.21	110.40
1	A	11	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	246	ALA	N-CA-CB	-5.97	101.74	110.10
1	A	20	TYR	CB-CA-C	-5.96	98.47	110.40
1	A	250	ARG	CD-NE-CZ	-5.94	115.28	123.60
1	A	38	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	148	ALA	N-CA-CB	5.90	118.36	110.10
1	A	394	ASN	N-CA-CB	5.90	121.22	110.60
1	A	400	PRO	N-CA-CB	5.88	110.36	103.30
1	A	391	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	351	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	180	ASP	CB-CA-C	5.78	121.97	110.40
1	A	139	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	312	TRP	CG-CD2-CE3	-5.71	128.76	133.90
1	A	156	ALA	CB-CA-C	-5.68	101.59	110.10
1	A	212	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	230	VAL	CA-CB-CG1	-5.62	102.48	110.90
1	A	153	PRO	N-CA-CB	5.61	110.03	103.30
1	A	402	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	185	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	A	226	ASP	CB-CG-OD1	-5.55	113.31	118.30
1	A	355	TRP	N-CA-CB	-5.53	100.65	110.60
1	A	261	ASP	CB-CG-OD1	5.52	123.26	118.30
1	A	276	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	414	TRP	N-CA-CB	5.51	120.51	110.60
1	A	187	TYR	CG-CD1-CE1	5.50	125.70	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	333	TYR	N-CA-CB	-5.46	100.77	110.60
1	A	367	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	176	ASN	CB-CA-C	5.43	121.26	110.40
1	A	312	TRP	N-CA-CB	-5.41	100.86	110.60
1	A	80	ASN	CB-CA-C	5.40	121.19	110.40
1	A	214	LEU	CB-CA-C	5.39	120.44	110.20
1	A	384	TYR	N-CA-CB	5.38	120.28	110.60
1	A	334	ALA	CB-CA-C	-5.37	102.05	110.10
1	A	239	TYR	CB-CG-CD1	5.32	124.19	121.00
1	A	375	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	198	GLU	N-CA-CB	5.29	120.12	110.60
1	A	256	TYR	CB-CA-C	-5.28	99.83	110.40
1	A	312	TRP	CB-CG-CD2	-5.28	119.73	126.60
1	A	253	ARG	N-CA-C	-5.25	96.81	111.00
1	A	128	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	336	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	226	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	154	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	A	121	ASN	C-N-CA	-5.15	108.83	121.70
1	A	185	TYR	N-CA-C	5.14	124.88	111.00
1	A	322	ASP	N-CA-CB	5.12	119.82	110.60
1	A	250	ARG	N-CA-CB	5.12	119.81	110.60
1	A	254	ASN	CB-CG-OD1	-5.11	111.38	121.60
1	A	124	GLU	CB-CA-C	5.11	120.62	110.40
1	A	125	LEU	CA-CB-CG	-5.10	103.57	115.30
1	A	260	LYS	CB-CA-C	-5.08	100.24	110.40
1	A	191	MET	CG-SD-CE	-5.08	92.08	100.20
1	A	11	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	133	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	A	22	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3245	0	2919	386	0
2	A	42	0	39	10	0
3	A	38	0	0	12	0
All	All	3325	0	2958	387	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 62.

All (387) 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	1.34	1.09
1:A:329:PRO:HA	1:A:386:HIS:HB2	1.39	0.99
1:A:77:PRO:HD3	1:A:278:TYR:CE2	2.01	0.96
1:A:168:ASN:HD21	2:A:1681:NAG:HN2	1.15	0.93
1:A:262:CYS:HB2	1:A:268:CYS:HA	1.52	0.92
1:A:173:LEU:HD23	1:A:331:LEU:CD2	1.99	0.92
1:A:77:PRO:HD3	1:A:278:TYR:HE2	1.34	0.91
1:A:95:GLN:HG2	1:A:96:PRO:CD	2.01	0.91
1:A:173:LEU:HD23	1:A:331:LEU:HD23	1.54	0.89
1:A:10:ILE:H	1:A:10:ILE:HD12	1.38	0.88
1:A:262:CYS:CB	1:A:268:CYS:HA	2.02	0.88
1:A:10:ILE:HG22	1:A:11:ASP:H	1.36	0.88
1:A:329:PRO:CA	1:A:386:HIS:HB2	2.03	0.88
1:A:355:TRP:CH2	1:A:357:TYR:HB2	2.10	0.87
1:A:279:LEU:HD23	1:A:295:TYR:CE1	2.10	0.86
1:A:328:LEU:HD23	1:A:329:PRO:HD2	1.57	0.85
1:A:21:LEU:HD23	1:A:125:LEU:HB2	1.56	0.85
1:A:191:MET:HG2	1:A:342:ASN:ND2	1.91	0.85
1:A:355:TRP:CZ2	1:A:357:TYR:HB2	2.11	0.85
1:A:71:ILE:HD13	1:A:278:TYR:CG	2.13	0.83
1:A:48:LEU:HD12	1:A:49:TRP:N	1.92	0.83
1:A:34:THR:HG22	1:A:35:PHE:H	1.44	0.82
1:A:180:ASP:HB2	1:A:317:HIS:HB3	1.59	0.82
1:A:26:GLU:CB	1:A:28:LYS:HD2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HG3	1:A:86:SER:HA	1.62	0.81
1:A:20:TYR:HE1	1:A:290:ALA:HA	1.45	0.81
1:A:93:LEU:HD12	1:A:94:ASP:H	1.45	0.80
1:A:50:LEU:HD22	1:A:95:GLN:HE22	1.44	0.80
1:A:320:VAL:HG12	1:A:353:LEU:HD21	1.62	0.80
1:A:189:GLU:HB3	1:A:190:PRO:HD3	1.64	0.79
1:A:65:ALA:O	1:A:400:PRO:HB2	1.83	0.79
1:A:420:SER:O	1:A:421:LEU:HD23	1.82	0.79
1:A:10:ILE:O	1:A:12:PRO:HD3	1.84	0.78
1:A:373:ILE:HD12	1:A:409:SER:OG	1.84	0.78
1:A:84:TRP:CZ2	1:A:411:VAL:HG21	2.18	0.78
1:A:48:LEU:HB3	1:A:142:ILE:HG23	1.66	0.77
1:A:378:ALA:HB1	1:A:406:ASN:HD22	1.50	0.77
1:A:29:HIS:O	1:A:102:SER:HB3	1.83	0.76
1:A:168:ASN:ND2	2:A:1681:NAG:HN2	1.84	0.76
1:A:37:SER:HB2	1:A:88:ALA:CA	2.16	0.76
1:A:56:CYS:HB3	3:A:472:HOH:O	1.87	0.75
1:A:162:HIS:N	1:A:162:HIS:ND1	2.30	0.75
1:A:390:LEU:CD2	1:A:410:MET:HG3	2.17	0.75
1:A:89:THR:HG22	3:A:461:HOH:O	1.86	0.74
1:A:45:PRO:HB3	1:A:139:ASP:HB2	1.70	0.74
1:A:125:LEU:HD23	1:A:125:LEU:N	2.02	0.74
1:A:93:LEU:HD12	1:A:94:ASP:N	2.03	0.73
1:A:95:GLN:HG2	1:A:96:PRO:HD3	1.68	0.73
1:A:96:PRO:N	1:A:99:VAL:HG21	2.02	0.73
1:A:37:SER:HB2	1:A:88:ALA:C	2.09	0.73
1:A:180:ASP:HB2	1:A:317:HIS:CB	2.19	0.72
1:A:133:TYR:O	1:A:138:GLN:HB2	1.89	0.72
1:A:366:VAL:HA	1:A:381:VAL:O	1.89	0.72
1:A:257:ASP:HA	1:A:337:LYS:O	1.90	0.72
1:A:191:MET:HG2	1:A:342:ASN:HD21	1.55	0.72
1:A:369:TRP:CZ3	1:A:378:ALA:HB3	2.24	0.72
1:A:283:TYR:O	1:A:286:GLU:HB2	1.88	0.71
1:A:171:SER:HA	1:A:328:LEU:HD21	1.70	0.71
1:A:34:THR:HG22	1:A:35:PHE:N	2.05	0.71
1:A:329:PRO:HA	1:A:386:HIS:O	1.89	0.71
1:A:10:ILE:HG22	1:A:11:ASP:N	2.04	0.71
1:A:368:ASN:ND2	2:A:3681:NAG:HN2	1.87	0.71
1:A:352:VAL:O	1:A:354:PRO:HD3	1.91	0.71
1:A:84:TRP:CH2	1:A:411:VAL:HG21	2.26	0.71
1:A:20:TYR:CE1	1:A:290:ALA:HA	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PRO:HA	3:A:461:HOH:O	1.91	0.69
1:A:18:THR:HG21	1:A:33:TRP:CD2	2.28	0.68
1:A:337:LYS:N	1:A:395:GLY:O	2.26	0.68
1:A:253:ARG:HH11	1:A:253:ARG:HB2	1.59	0.68
1:A:347:LYS:O	1:A:350:THR:HG22	1.94	0.68
1:A:282:ASP:O	1:A:286:GLU:HG2	1.93	0.67
1:A:327:ASP:OD1	1:A:356:LYS:NZ	2.28	0.67
2:A:3681:NAG:H82	2:A:3681:NAG:O3	1.95	0.67
1:A:72:GLY:O	1:A:75:LEU:N	2.26	0.67
1:A:12:PRO:O	1:A:14:VAL:N	2.28	0.66
1:A:48:LEU:HD12	1:A:49:TRP:H	1.58	0.66
1:A:249:GLN:HA	3:A:483:HOH:O	1.95	0.66
1:A:180:ASP:HB2	1:A:317:HIS:CG	2.30	0.65
1:A:18:THR:HG22	1:A:33:TRP:HA	1.77	0.65
1:A:5:PRO:O	1:A:8:LEU:N	2.27	0.65
1:A:353:LEU:HG	1:A:354:PRO:N	2.11	0.65
1:A:60:THR:O	1:A:64:PHE:HB3	1.97	0.65
1:A:95:GLN:HG2	1:A:96:PRO:N	2.08	0.65
1:A:345:GLY:HA3	3:A:471:HOH:O	1.96	0.64
1:A:116:GLY:O	1:A:119:VAL:N	2.28	0.64
1:A:202:LEU:HD23	1:A:206:GLU:HB3	1.80	0.64
1:A:94:ASP:OD2	1:A:101:PHE:N	2.24	0.64
1:A:304:ARG:NH1	1:A:305:ASN:OD1	2.31	0.64
1:A:406:ASN:O	1:A:409:SER:HB2	1.99	0.63
1:A:354:PRO:O	1:A:355:TRP:HB3	1.98	0.63
1:A:50:LEU:HD22	1:A:95:GLN:NE2	2.13	0.63
1:A:75:LEU:HD21	1:A:277:ASP:HB3	1.80	0.63
1:A:8:LEU:HD13	1:A:10:ILE:CD1	2.29	0.63
1:A:140:PHE:HB3	1:A:168:ASN:O	1.98	0.63
1:A:181:PRO:HD2	1:A:225:TYR:OH	1.99	0.63
1:A:373:ILE:HG22	1:A:374:THR:N	2.14	0.63
1:A:125:LEU:O	1:A:128:ASP:HB2	1.98	0.63
1:A:330:ILE:N	1:A:386:HIS:O	2.31	0.62
1:A:181:PRO:O	1:A:185:TYR:HB2	1.98	0.62
1:A:38:ARG:HG2	1:A:85:ASN:O	1.98	0.62
1:A:335:GLY:CA	1:A:395:GLY:HA3	2.29	0.62
1:A:305:ASN:OD1	1:A:305:ASN:N	2.30	0.62
1:A:85:ASN:HB2	1:A:88:ALA:O	2.00	0.62
1:A:270:PRO:HD2	3:A:484:HOH:O	2.00	0.61
1:A:39:ASN:HB3	1:A:44:ASP:OD2	2.00	0.61
1:A:31:PHE:O	1:A:93:LEU:HD12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD11	1:A:328:LEU:HD12	1.82	0.61
1:A:166:ASN:OD1	1:A:167:PHE:HD1	1.84	0.61
1:A:360:GLU:O	1:A:363:SER:N	2.26	0.61
1:A:259:ARG:HD3	1:A:337:LYS:CD	2.22	0.60
1:A:123:LEU:HB3	1:A:167:PHE:CZ	2.36	0.60
1:A:57:SER:HB2	1:A:100:GLY:HA3	1.83	0.60
1:A:361:PHE:CE1	1:A:382:LYS:HD2	2.37	0.60
1:A:131:PRO:HD2	1:A:132:GLU:OE2	2.02	0.60
1:A:143:ALA:CB	1:A:173:LEU:HB2	2.32	0.60
1:A:127:PHE:HD2	1:A:167:PHE:CD1	2.20	0.59
1:A:30:PHE:CZ	1:A:118:ASP:HB3	2.36	0.59
1:A:95:GLN:CB	1:A:96:PRO:HA	2.30	0.59
1:A:71:ILE:HD13	1:A:278:TYR:CD2	2.38	0.58
1:A:336:ASP:OD1	1:A:337:LYS:HE2	2.02	0.58
1:A:180:ASP:OD2	1:A:183:THR:HB	2.03	0.58
1:A:182:LEU:HB2	1:A:221:ILE:CG2	2.33	0.58
1:A:274:ASP:O	1:A:277:ASP:HB2	2.02	0.58
1:A:304:ARG:HG2	1:A:305:ASN:OD1	2.04	0.58
1:A:121:ASN:O	1:A:125:LEU:HG	2.03	0.57
1:A:191:MET:HE3	1:A:338:ASP:O	2.03	0.57
1:A:5:PRO:HD2	1:A:16:GLN:O	2.05	0.57
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.87	0.57
1:A:71:ILE:HG21	1:A:278:TYR:HB2	1.87	0.57
1:A:279:LEU:O	1:A:285:LYS:HG2	2.05	0.57
1:A:172:VAL:HG22	1:A:330:ILE:HG12	1.87	0.57
1:A:143:ALA:HB2	1:A:173:LEU:HB2	1.86	0.56
1:A:186:ASN:H	1:A:186:ASN:ND2	2.03	0.56
1:A:21:LEU:HD23	1:A:125:LEU:CB	2.32	0.56
1:A:173:LEU:HD23	1:A:331:LEU:HD22	1.83	0.56
1:A:328:LEU:HD23	1:A:329:PRO:CD	2.34	0.56
1:A:335:GLY:HA2	1:A:395:GLY:HA3	1.86	0.56
1:A:44:ASP:HB3	1:A:88:ALA:HA	1.85	0.56
1:A:127:PHE:HD2	1:A:167:PHE:CG	2.23	0.56
1:A:176:ASN:HB2	3:A:458:HOH:O	2.05	0.56
1:A:378:ALA:CB	1:A:406:ASN:HD22	2.18	0.56
1:A:10:ILE:N	1:A:10:ILE:HD12	2.14	0.56
1:A:146:SER:CA	1:A:177:GLY:HA2	2.36	0.56
1:A:63:PHE:HA	1:A:69:SER:O	2.05	0.56
1:A:77:PRO:O	1:A:78:ILE:HG13	2.05	0.56
1:A:30:PHE:HZ	1:A:118:ASP:HB3	1.70	0.56
1:A:320:VAL:HG12	1:A:353:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HD11	1:A:169:LEU:HB2	1.86	0.56
1:A:268:CYS:HB2	3:A:482:HOH:O	2.05	0.55
1:A:410:MET:CE	1:A:411:VAL:HG23	2.36	0.55
1:A:127:PHE:CD2	1:A:167:PHE:CG	2.94	0.55
1:A:198:GLU:OE2	1:A:259:ARG:HG2	2.06	0.55
1:A:254:ASN:OD1	1:A:268:CYS:HB3	2.07	0.55
1:A:413:GLU:O	1:A:413:GLU:HG3	2.05	0.55
1:A:158:GLU:O	1:A:161:SER:HB2	2.06	0.55
1:A:28:LYS:HE2	1:A:118:ASP:OD2	2.07	0.55
1:A:253:ARG:HD2	1:A:260:LYS:O	2.07	0.55
1:A:159:ILE:C	1:A:161:SER:H	2.10	0.55
1:A:146:SER:HA	1:A:177:GLY:HA2	1.89	0.54
1:A:350:THR:HG21	1:A:389:TYR:HB2	1.89	0.54
1:A:53:GLY:HA3	1:A:54:PRO:C	2.27	0.54
1:A:78:ILE:O	1:A:78:ILE:HG22	2.07	0.54
1:A:355:TRP:O	1:A:358:ASP:HB2	2.08	0.54
1:A:148:ALA:O	1:A:152:ILE:HG13	2.08	0.54
1:A:32:PHE:N	1:A:32:PHE:CD1	2.76	0.54
1:A:148:ALA:HA	1:A:151:TYR:CD2	2.43	0.53
1:A:159:ILE:HD13	1:A:169:LEU:HD22	1.90	0.53
1:A:159:ILE:O	1:A:161:SER:N	2.41	0.53
1:A:68:PRO:O	1:A:80:ASN:N	2.42	0.53
1:A:154:VAL:HG21	1:A:316:TYR:CD1	2.43	0.53
1:A:317:HIS:H	1:A:317:HIS:CD2	2.27	0.53
1:A:198:GLU:HG3	1:A:199:PRO:HD2	1.91	0.53
1:A:106:SER:O	1:A:106:SER:OG	2.27	0.53
1:A:216:ARG:HG2	1:A:239:TYR:CZ	2.44	0.52
1:A:109:VAL:O	1:A:109:VAL:HG23	2.09	0.52
1:A:8:LEU:HD13	1:A:10:ILE:HD13	1.91	0.52
1:A:180:ASP:CB	1:A:317:HIS:HB3	2.35	0.52
1:A:10:ILE:H	1:A:10:ILE:CD1	2.17	0.52
1:A:220:LEU:HD13	1:A:236:ALA:HA	1.91	0.52
1:A:189:GLU:HB3	1:A:190:PRO:CD	2.36	0.52
1:A:410:MET:HE3	1:A:411:VAL:HG23	1.90	0.52
1:A:130:PHE:C	1:A:132:GLU:H	2.13	0.52
1:A:146:SER:HA	1:A:176:ASN:O	2.10	0.52
1:A:126:PHE:HE1	1:A:127:PHE:CE1	2.28	0.52
1:A:12:PRO:C	1:A:14:VAL:H	2.12	0.52
1:A:62:LEU:HD23	1:A:62:LEU:C	2.30	0.52
1:A:15:THR:O	1:A:36:GLU:HG3	2.09	0.52
1:A:62:LEU:HB2	1:A:92:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:SER:O	1:A:408:LEU:HD22	2.09	0.51
1:A:182:LEU:HB2	1:A:221:ILE:HG21	1.93	0.51
1:A:378:ALA:HB1	1:A:406:ASN:ND2	2.23	0.51
1:A:380:GLU:N	1:A:391:ARG:O	2.44	0.51
1:A:329:PRO:CB	1:A:386:HIS:HB2	2.39	0.51
1:A:261:ASP:OD1	1:A:261:ASP:N	2.44	0.51
1:A:317:HIS:N	1:A:317:HIS:CD2	2.78	0.51
1:A:224:CYS:O	1:A:228:GLN:N	2.33	0.51
1:A:155:PHE:CD1	1:A:155:PHE:N	2.78	0.51
1:A:403:VAL:O	1:A:403:VAL:HG23	2.11	0.51
1:A:202:LEU:HD22	1:A:210:MET:HE1	1.94	0.50
1:A:141:HIS:N	1:A:141:HIS:CD2	2.79	0.50
1:A:206:GLU:OE2	1:A:247:PRO:HB3	2.10	0.50
1:A:153:PRO:O	1:A:156:ALA:HB3	2.11	0.50
1:A:202:LEU:CD2	1:A:206:GLU:HB3	2.42	0.50
1:A:95:GLN:HG2	1:A:96:PRO:CG	2.42	0.50
1:A:168:ASN:ND2	2:A:1681:NAG:C1	2.75	0.50
1:A:217:CYS:HB2	1:A:239:TYR:HD2	1.76	0.50
1:A:50:LEU:N	1:A:143:ALA:O	2.41	0.50
1:A:217:CYS:HB2	1:A:239:TYR:CD2	2.46	0.50
1:A:174:ILE:HG22	1:A:174:ILE:O	2.11	0.50
1:A:130:PHE:N	1:A:131:PRO:HD3	2.27	0.49
1:A:18:THR:CG2	1:A:33:TRP:HA	2.42	0.49
1:A:191:MET:CE	1:A:342:ASN:ND2	2.75	0.49
1:A:171:SER:HA	1:A:328:LEU:CD2	2.40	0.49
1:A:247:PRO:HA	1:A:250:ARG:HG3	1.94	0.49
1:A:34:THR:CG2	1:A:35:PHE:H	2.22	0.49
1:A:182:LEU:HB3	1:A:225:TYR:CE2	2.48	0.49
1:A:323:LEU:O	1:A:326:GLN:N	2.42	0.49
1:A:55:GLY:O	1:A:298:CYS:HA	2.12	0.49
1:A:72:GLY:O	1:A:74:ASP:N	2.46	0.49
1:A:378:ALA:CB	1:A:406:ASN:ND2	2.76	0.49
1:A:21:LEU:CD2	1:A:126:PHE:H	2.25	0.49
1:A:20:TYR:CE2	1:A:31:PHE:HB2	2.48	0.49
1:A:368:ASN:OD1	2:A:3681:NAG:O5	2.29	0.49
1:A:390:LEU:HD22	1:A:410:MET:HG3	1.92	0.49
1:A:234:VAL:HB	1:A:235:PRO:CD	2.43	0.48
1:A:279:LEU:CD1	1:A:279:LEU:N	2.76	0.48
1:A:34:THR:HG23	1:A:90:VAL:O	2.12	0.48
1:A:100:GLY:CA	1:A:295:TYR:CE2	2.96	0.48
1:A:23:VAL:HG11	1:A:30:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:HB3	1:A:171:SER:O	2.13	0.48
1:A:214:LEU:O	1:A:217:CYS:N	2.47	0.48
1:A:279:LEU:HD23	1:A:295:TYR:CZ	2.48	0.48
1:A:292:VAL:HG13	1:A:293:ASP:N	2.29	0.48
1:A:9:GLY:O	1:A:10:ILE:O	2.31	0.48
1:A:134:VAL:O	1:A:136:LYS:N	2.46	0.48
1:A:95:GLN:HG2	1:A:96:PRO:CA	2.43	0.48
1:A:46:VAL:HG22	1:A:89:THR:HG23	1.96	0.48
1:A:102:SER:O	1:A:103:TYR:HB3	2.12	0.48
1:A:284:VAL:O	1:A:288:VAL:HG23	2.13	0.47
1:A:368:ASN:ND2	2:A:3681:NAG:C1	2.77	0.47
1:A:399:VAL:N	1:A:400:PRO:CD	2.77	0.47
1:A:48:LEU:C	1:A:48:LEU:HD12	2.27	0.47
1:A:182:LEU:HB2	1:A:221:ILE:HG22	1.95	0.47
1:A:286:GLU:HA	1:A:286:GLU:OE1	2.15	0.47
1:A:369:TRP:CE3	1:A:378:ALA:HB3	2.50	0.47
1:A:80:ASN:HA	1:A:81:PRO:HD3	1.66	0.47
1:A:100:GLY:HA2	1:A:295:TYR:CE2	2.50	0.47
1:A:370:THR:CG2	1:A:371:ALA:N	2.78	0.47
1:A:389:TYR:HD2	3:A:469:HOH:O	1.97	0.47
1:A:87:ASN:ND2	2:A:871:NAG:C1	2.77	0.47
1:A:65:ALA:O	1:A:400:PRO:O	2.32	0.47
1:A:80:ASN:OD1	1:A:81:PRO:HD2	2.15	0.47
1:A:87:ASN:HD21	2:A:871:NAG:C1	2.27	0.47
1:A:22:ASP:OD2	1:A:29:HIS:ND1	2.44	0.47
1:A:253:ARG:CB	1:A:253:ARG:HH11	2.27	0.47
1:A:122:PHE:CD1	1:A:122:PHE:C	2.89	0.47
1:A:407:ALA:HB3	3:A:462:HOH:O	2.15	0.47
1:A:185:TYR:OH	1:A:241:ASN:ND2	2.47	0.46
1:A:21:LEU:HD23	1:A:126:PHE:H	1.80	0.46
1:A:247:PRO:O	1:A:250:ARG:HG3	2.16	0.46
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.55	0.46
1:A:368:ASN:ND2	2:A:3681:NAG:N2	2.60	0.46
1:A:50:LEU:CD2	1:A:95:GLN:HE22	2.21	0.46
1:A:10:ILE:N	1:A:10:ILE:CD1	2.78	0.46
1:A:188:TYR:CB	1:A:244:GLN:HG2	2.45	0.46
1:A:213:SER:CB	1:A:243:ALA:HB1	2.46	0.46
1:A:304:ARG:HG3	1:A:308:PHE:CD2	2.51	0.46
1:A:18:THR:HG21	1:A:33:TRP:CG	2.50	0.46
1:A:86:SER:CB	1:A:408:LEU:HD21	2.46	0.46
1:A:188:TYR:HB2	1:A:244:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:CE2	1:A:411:VAL:HG21	2.50	0.46
1:A:95:GLN:CG	1:A:96:PRO:HA	2.46	0.46
1:A:183:THR:O	1:A:186:ASN:ND2	2.49	0.46
1:A:23:VAL:HG13	1:A:28:LYS:HB2	1.97	0.46
1:A:304:ARG:HG3	1:A:308:PHE:HD2	1.81	0.46
1:A:335:GLY:HA3	1:A:395:GLY:C	2.36	0.46
1:A:50:LEU:CD2	1:A:95:GLN:NE2	2.79	0.46
1:A:335:GLY:HA3	1:A:395:GLY:HA3	1.96	0.46
1:A:253:ARG:NE	1:A:258:ILE:O	2.49	0.46
1:A:340:ILE:CG2	1:A:341:CYS:N	2.79	0.46
1:A:328:LEU:HD23	1:A:328:LEU:C	2.36	0.45
1:A:340:ILE:HG23	1:A:341:CYS:N	2.31	0.45
1:A:8:LEU:HD13	1:A:10:ILE:HD11	1.98	0.45
1:A:136:LYS:HB2	1:A:138:GLN:OE1	2.16	0.45
1:A:378:ALA:O	1:A:393:PHE:HB2	2.17	0.45
1:A:186:ASN:HB3	1:A:214:LEU:HD21	1.97	0.45
1:A:20:TYR:C	1:A:21:LEU:HD12	2.37	0.45
1:A:18:THR:CG2	1:A:33:TRP:CD2	2.98	0.45
1:A:5:PRO:O	1:A:8:LEU:HB2	2.16	0.45
1:A:123:LEU:HD11	1:A:140:PHE:CZ	2.52	0.45
1:A:147:TYR:C	1:A:149:GLY:H	2.18	0.45
1:A:71:ILE:HD13	1:A:278:TYR:CB	2.45	0.45
1:A:58:SER:HB2	1:A:93:LEU:O	2.17	0.45
1:A:198:GLU:CG	1:A:199:PRO:HD2	2.46	0.44
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.63	0.44
1:A:355:TRP:CZ3	1:A:357:TYR:HD2	2.35	0.44
1:A:369:TRP:CZ3	1:A:378:ALA:CB	2.99	0.44
1:A:159:ILE:CD1	1:A:169:LEU:HB2	2.47	0.44
1:A:348:ALA:HA	1:A:351:ASP:HB2	1.99	0.44
1:A:21:LEU:CD1	1:A:21:LEU:N	2.75	0.44
1:A:182:LEU:CB	1:A:225:TYR:CE2	3.00	0.44
1:A:320:VAL:CG1	1:A:353:LEU:CD2	2.95	0.44
1:A:350:THR:HG1	1:A:387:PHE:HZ	1.62	0.44
1:A:74:ASP:O	1:A:76:LYS:HG2	2.17	0.44
1:A:126:PHE:CD1	1:A:126:PHE:C	2.90	0.44
1:A:234:VAL:CB	1:A:235:PRO:CD	2.96	0.44
1:A:321:THR:HG23	1:A:354:PRO:O	2.17	0.44
1:A:5:PRO:HB3	1:A:33:TRP:CZ2	2.52	0.44
1:A:134:VAL:O	1:A:137:GLY:N	2.50	0.44
1:A:355:TRP:CH2	1:A:357:TYR:HD2	2.36	0.44
1:A:126:PHE:CE1	1:A:127:PHE:CE1	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HB3	1:A:269:TYR:H	1.82	0.43
1:A:324:LEU:HB3	1:A:355:TRP:CE3	2.54	0.43
1:A:62:LEU:HB2	1:A:92:PHE:CD1	2.53	0.43
1:A:130:PHE:N	1:A:130:PHE:CD1	2.87	0.43
1:A:143:ALA:HB1	1:A:173:LEU:HB2	2.00	0.43
1:A:421:LEU:HA	1:A:421:LEU:HD23	1.64	0.43
1:A:5:PRO:HG2	1:A:16:GLN:CB	2.49	0.43
1:A:338:ASP:OD1	1:A:339:PHE:N	2.52	0.43
1:A:136:LYS:HA	1:A:136:LYS:HD2	1.74	0.43
1:A:248:TYR:CE1	1:A:258:ILE:HG13	2.54	0.43
1:A:329:PRO:HB3	1:A:386:HIS:HB2	2.00	0.43
1:A:57:SER:HB2	1:A:100:GLY:CA	2.48	0.43
1:A:108:GLY:O	1:A:109:VAL:HG22	2.18	0.43
1:A:147:TYR:C	1:A:149:GLY:N	2.72	0.43
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.36	0.43
1:A:46:VAL:HG21	1:A:133:TYR:HB3	2.00	0.43
1:A:123:LEU:HA	1:A:123:LEU:HD23	1.74	0.43
1:A:270:PRO:O	1:A:273:GLN:N	2.48	0.43
1:A:271:THR:HA	1:A:274:ASP:OD2	2.19	0.43
1:A:202:LEU:CD2	1:A:210:MET:HE1	2.49	0.42
1:A:141:HIS:HD1	1:A:171:SER:HG	1.67	0.42
1:A:321:THR:OG1	1:A:354:PRO:O	2.30	0.42
1:A:39:ASN:HB3	1:A:40:ASP:H	1.62	0.42
1:A:248:TYR:OH	1:A:258:ILE:HA	2.19	0.42
1:A:93:LEU:CD1	1:A:94:ASP:N	2.79	0.42
1:A:91:ILE:HG22	1:A:92:PHE:N	2.34	0.42
1:A:95:GLN:HG3	3:A:476:HOH:O	2.19	0.42
1:A:348:ALA:O	1:A:352:VAL:HG22	2.19	0.42
1:A:4:ASP:C	1:A:6:LYS:N	2.72	0.42
1:A:146:SER:O	1:A:177:GLY:HA2	2.20	0.42
1:A:262:CYS:HB3	1:A:268:CYS:HA	1.96	0.42
1:A:186:ASN:N	1:A:186:ASN:ND2	2.68	0.42
1:A:38:ARG:HG3	1:A:86:SER:CA	2.43	0.42
1:A:135:ASN:C	1:A:137:GLY:H	2.23	0.42
1:A:171:SER:HB3	1:A:329:PRO:HG2	2.01	0.42
1:A:182:LEU:HB3	1:A:225:TYR:HE2	1.84	0.42
1:A:129:GLN:C	1:A:131:PRO:HD3	2.41	0.41
1:A:155:PHE:O	1:A:159:ILE:HG22	2.20	0.41
1:A:320:VAL:CG1	1:A:324:LEU:HD12	2.50	0.41
1:A:71:ILE:CD1	1:A:278:TYR:CG	2.94	0.41
1:A:69:SER:HA	1:A:78:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:HB2	1:A:166:ASN:OD1	2.20	0.41
1:A:146:SER:OG	1:A:147:TYR:N	2.53	0.41
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.83	0.41
1:A:21:LEU:HD21	1:A:126:PHE:N	2.35	0.41
1:A:276:ASP:OD1	1:A:295:TYR:CE1	2.73	0.41
1:A:295:TYR:C	1:A:295:TYR:CD1	2.94	0.41
1:A:342:ASN:HB2	3:A:471:HOH:O	2.19	0.41
1:A:407:ALA:O	1:A:411:VAL:N	2.35	0.41
1:A:244:GLN:HE21	1:A:244:GLN:HB2	1.32	0.41
1:A:390:LEU:HD23	1:A:410:MET:HG3	2.00	0.41
1:A:10:ILE:CG2	1:A:11:ASP:N	2.79	0.41
1:A:392:VAL:HG12	1:A:392:VAL:O	2.19	0.41
1:A:80:ASN:C	1:A:82:TYR:H	2.23	0.41
1:A:142:ILE:HG22	1:A:143:ALA:N	2.36	0.41
1:A:155:PHE:HD1	1:A:155:PHE:N	2.18	0.41
1:A:202:LEU:CD2	1:A:210:MET:CE	2.98	0.41
1:A:292:VAL:CG1	1:A:293:ASP:N	2.81	0.41
1:A:325:ASN:OD1	1:A:356:LYS:N	2.48	0.41
1:A:191:MET:CE	1:A:342:ASN:HD22	2.33	0.41
1:A:240:CYS:C	1:A:242:ASN:N	2.74	0.41
1:A:242:ASN:O	1:A:246:ALA:HB3	2.20	0.41
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.72	0.41
1:A:127:PHE:HA	1:A:127:PHE:HD1	1.67	0.41
1:A:48:LEU:HD13	1:A:48:LEU:HA	1.53	0.41
1:A:54:PRO:HG3	1:A:147:TYR:CE2	2.56	0.41
1:A:112:THR:HG22	1:A:154:VAL:HG11	2.02	0.40
1:A:130:PHE:HB3	1:A:133:TYR:CE2	2.56	0.40
1:A:214:LEU:HD11	1:A:218:LEU:HD21	2.03	0.40
1:A:322:ASP:O	1:A:326:GLN:N	2.55	0.40
1:A:358:ASP:HB3	1:A:359:GLU:H	1.74	0.40
1:A:247:PRO:HA	1:A:250:ARG:CG	2.51	0.40
1:A:384:TYR:CE1	1:A:385:LYS:CG	3.04	0.40
1:A:82:TYR:HB2	1:A:404:PRO:HB2	2.03	0.40
1:A:130:PHE:N	1:A:131:PRO:CD	2.85	0.40
1:A:84:TRP:CZ2	1:A:411:VAL:CG2	2.96	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	419/421 (100%)	326 (78%)	64 (15%)	29 (7%)	1 1

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	12	PRO
1	A	13	ASN
1	A	14	VAL
1	A	15	THR
1	A	24	GLU
1	A	125	LEU
1	A	135	ASN
1	A	266	ASN
1	A	342	ASN
1	A	358	ASP
1	A	98	ASN
1	A	311	ASP
1	A	397	HIS
1	A	73	PRO
1	A	126	PHE
1	A	6	LYS
1	A	64	PHE
1	A	77	PRO
1	A	136	LYS
1	A	185	TYR
1	A	88	ALA
1	A	300	PHE
1	A	411	VAL
1	A	312	TRP
1	A	131	PRO
1	A	9	GLY
1	A	134	VAL

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Mol	Chain	Res	Type
1	A	354	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	332/363 (92%)	251 (76%)	81 (24%)	0 1

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	10	ILE
1	A	33	TRP
1	A	37	SER
1	A	38	ARG
1	A	47	ILE
1	A	48	LEU
1	A	51	ASN
1	A	62	LEU
1	A	66	LEU
1	A	70	SER
1	A	87	ASN
1	A	89	THR
1	A	94	ASP
1	A	95	GLN
1	A	97	VAL
1	A	106	SER
1	A	107	SER
1	A	111	ASN
1	A	112	THR
1	A	122	PHE
1	A	124	GLU
1	A	128	ASP
1	A	129	GLN
1	A	132	GLU

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Mol	Chain	Res	Type
1	A	134	VAL
1	A	135	ASN
1	A	141	HIS
1	A	157	SER
1	A	159	ILE
1	A	161	SER
1	A	162	HIS
1	A	164	ASP
1	A	165	ARG
1	A	166	ASN
1	A	170	THR
1	A	180	ASP
1	A	184	GLN
1	A	186	ASN
1	A	198	GLU
1	A	202	LEU
1	A	205	GLU
1	A	208	SER
1	A	216	ARG
1	A	217	CYS
1	A	223	SER
1	A	244	GLN
1	A	250	ARG
1	A	253	ARG
1	A	260	LYS
1	A	261	ASP
1	A	262	CYS
1	A	263	GLU
1	A	272	LEU
1	A	274	ASP
1	A	276	ASP
1	A	283	TYR
1	A	292	VAL
1	A	304	ARG
1	A	305	ASN
1	A	311	ASP
1	A	313	MET
1	A	314	LYS
1	A	326	GLN
1	A	331	LEU
1	A	340	ILE
1	A	350	THR

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Mol	Chain	Res	Type
1	A	356	LYS
1	A	363	SER
1	A	368	ASN
1	A	376	GLU
1	A	377	VAL
1	A	381	VAL
1	A	382	LYS
1	A	386	HIS
1	A	399	VAL
1	A	401	PHE
1	A	402	ASP
1	A	405	GLU
1	A	412	ASN
1	A	413	GLU

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

Mol	Chain	Res	Type
1	A	80	ASN
1	A	95	GLN
1	A	168	ASN
1	A	186	ASN
1	A	241	ASN
1	A	244	GLN
1	A	317	HIS
1	A	342	ASN
1	A	368	ASN
1	A	406	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 monosaccharides 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	-	14,14,15	2.07	6 (42%)	17,19,21	2.91	5 (29%)
2	NAG	A	871	-	14,14,15	1.87	4 (28%)	17,19,21	2.75	8 (47%)
2	NAG	A	3681	-	14,14,15	0.78	0	17,19,21	4.07	6 (35%)

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	-	-	6/6/23/26	0/1/1/1
2	NAG	A	871	-	-	3/6/23/26	0/1/1/1
2	NAG	A	3681	-	-	6/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1681	NAG	C2-N2	4.89	1.54	1.46
2	A	871	NAG	C1-C2	4.62	1.59	1.52
2	A	871	NAG	O5-C5	2.92	1.49	1.43
2	A	871	NAG	C3-C2	2.61	1.58	1.52
2	A	1681	NAG	C3-C2	2.60	1.58	1.52
2	A	871	NAG	C2-N2	2.51	1.50	1.46
2	A	1681	NAG	C1-C2	2.37	1.55	1.52
2	A	1681	NAG	O7-C7	2.33	1.28	1.23
2	A	1681	NAG	C4-C3	2.06	1.57	1.52
2	A	1681	NAG	C7-N2	2.03	1.41	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3681	NAG	O6-C6-C5	14.87	162.30	111.29
2	A	1681	NAG	O6-C6-C5	8.25	139.59	111.29
2	A	871	NAG	O6-C6-C5	6.95	135.14	111.29
2	A	1681	NAG	C2-N2-C7	5.92	131.33	122.90
2	A	871	NAG	C1-O5-C5	5.46	119.59	112.19
2	A	3681	NAG	O7-C7-C8	-5.03	112.72	122.06
2	A	1681	NAG	O7-C7-C8	-4.60	113.51	122.06
2	A	3681	NAG	O7-C7-N2	2.95	127.38	121.95
2	A	871	NAG	C1-C2-N2	2.87	115.40	110.49
2	A	871	NAG	O5-C5-C6	2.72	111.47	107.20
2	A	871	NAG	O7-C7-C8	-2.56	117.31	122.06
2	A	1681	NAG	O7-C7-N2	2.52	126.59	121.95
2	A	871	NAG	C3-C4-C5	2.49	114.69	110.24
2	A	3681	NAG	O5-C5-C6	-2.39	103.45	107.20
2	A	3681	NAG	C1-C2-N2	2.18	114.22	110.49
2	A	871	NAG	O5-C5-C4	2.15	116.06	110.83
2	A	1681	NAG	C1-O5-C5	-2.13	109.30	112.19
2	A	3681	NAG	C8-C7-N2	2.13	119.70	116.10
2	A	871	NAG	O7-C7-N2	2.09	125.79	121.95

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1681	NAG	C8-C7-N2-C2
2	A	1681	NAG	O7-C7-N2-C2
2	A	871	NAG	C3-C2-N2-C7
2	A	3681	NAG	C3-C2-N2-C7
2	A	3681	NAG	C8-C7-N2-C2
2	A	3681	NAG	O7-C7-N2-C2
2	A	871	NAG	C4-C5-C6-O6
2	A	3681	NAG	O5-C5-C6-O6
2	A	871	NAG	O5-C5-C6-O6
2	A	3681	NAG	C4-C5-C6-O6
2	A	1681	NAG	C4-C5-C6-O6
2	A	3681	NAG	C1-C2-N2-C7
2	A	1681	NAG	C1-C2-N2-C7
2	A	1681	NAG	O5-C5-C6-O6
2	A	1681	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1681	NAG	3	0
2	A	871	NAG	2	0
2	A	3681	NAG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.