



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:54 PM GMT

PDB ID : 1HRN  
Title : HIGH RESOLUTION CRYSTAL STRUCTURES OF RECOMBINANT HUMAN RENIN IN COMPLEX WITH POLYHYDROXYMONOAMIDE INHIBITORS  
Authors : Tong, L.; Anderson, P.C.  
Deposited on : 1995-03-31  
Resolution : 1.80 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

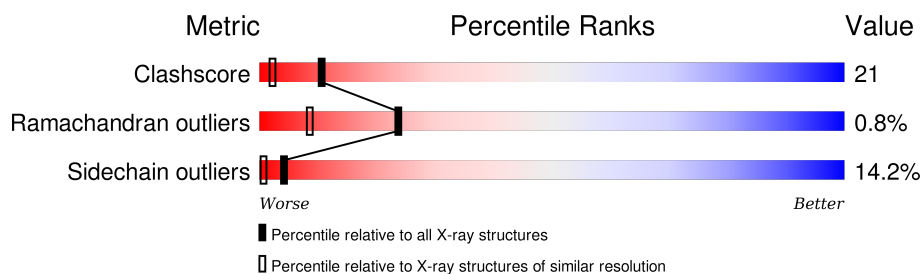
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5593 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 RENIN.

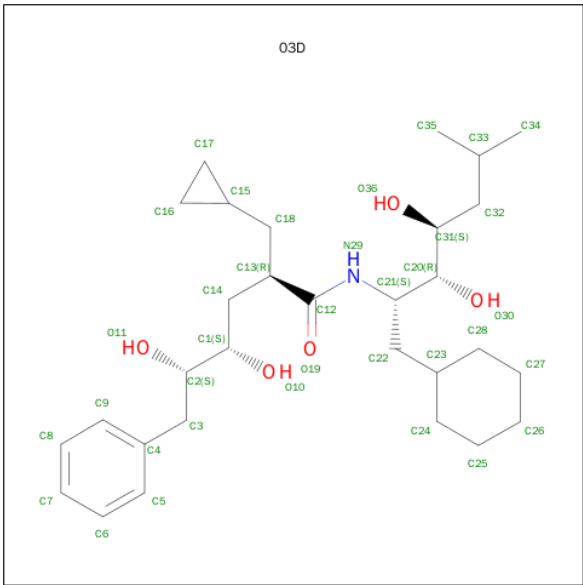
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	1
			2576	1644	417	501	14			
1	B	334	Total	C	N	O	S	0	0	1
			2551	1630	409	498	14			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (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	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (2R,4S,5S)-N-[(2S,3R,4S)-1-CYCLOHEXYL-3,4-DIHYDROXY-6-METHYLEHTAN-2-YL]-2-(CYCLOPROPYLMETHYL)-4,5-DIHYDROXY-6-PHENYLHEXANAMIDE (three-letter code: 03D) (formula:  $C_{30}H_{49}NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			36	30	1	5		
3	B	1	Total	C	N	O	0	0
			36	30	1	5		

- Molecule 4 is water.

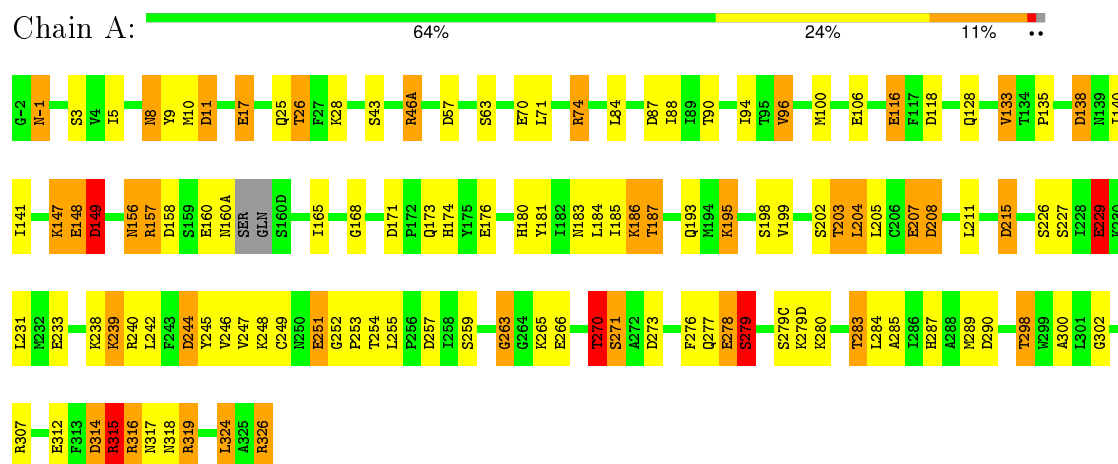
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	160	Total	O	0	0
			160	160		

### 3 Residue-property plots

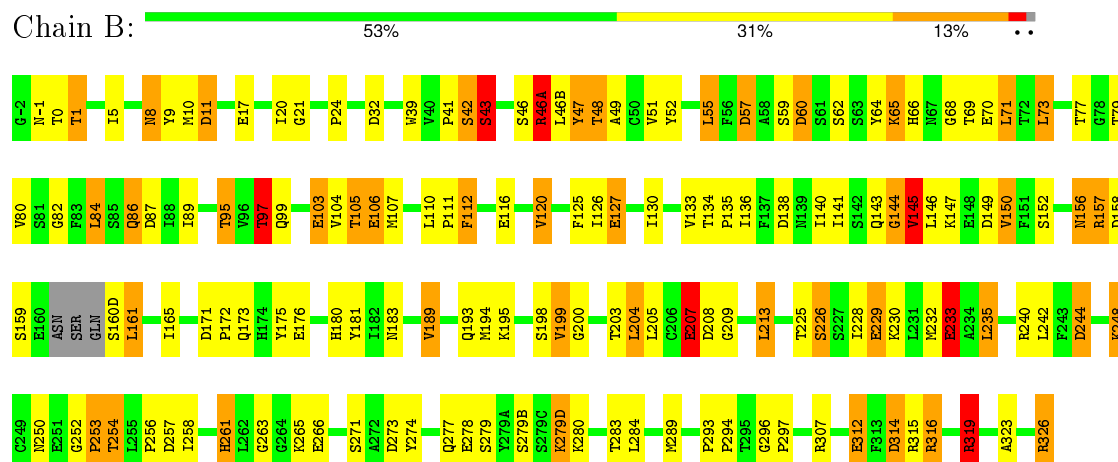
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: RENIN



#### • Molecule 1: RENIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.10 Å   141.10 Å   141.10 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	6.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, $R_{free}$	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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, O3D

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	1.17	15/2635 (0.6%)	1.51	38/3572 (1.1%)
1	B	1.17	14/2610 (0.5%)	1.57	40/3542 (1.1%)
All	All	1.17	29/5245 (0.6%)	1.54	78/7114 (1.1%)

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

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

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	GLU	CD-OE1	11.52	1.38	1.25
1	A	233	GLU	CD-OE1	9.49	1.36	1.25
1	A	229	GLU	CD-OE1	9.06	1.35	1.25
1	B	17	GLU	CD-OE2	9.04	1.35	1.25
1	B	207	GLU	CD-OE1	8.75	1.35	1.25
1	B	176	GLU	CD-OE2	8.06	1.34	1.25
1	A	207	GLU	CD-OE1	8.01	1.34	1.25
1	B	312	GLU	CD-OE2	-7.99	1.16	1.25
1	A	266	GLU	CD-OE2	7.94	1.34	1.25
1	B	229	GLU	CD-OE1	7.80	1.34	1.25
1	B	127	GLU	CD-OE1	7.55	1.33	1.25
1	B	266	GLU	CD-OE2	7.55	1.33	1.25
1	A	278	GLU	CD-OE2	7.46	1.33	1.25
1	B	103	GLU	CD-OE1	7.39	1.33	1.25
1	A	70	GLU	CD-OE1	7.33	1.33	1.25
1	A	160	GLU	CD-OE2	7.28	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	GLU	CD-OE1	7.07	1.33	1.25
1	A	74	ARG	CZ-NH2	7.03	1.42	1.33
1	B	70	GLU	CD-OE2	6.79	1.33	1.25
1	B	233	GLU	CD-OE1	6.76	1.33	1.25
1	A	176	GLU	CD-OE1	6.19	1.32	1.25
1	A	148	GLU	CD-OE1	6.15	1.32	1.25
1	A	312	GLU	CD-OE2	5.81	1.32	1.25
1	A	116	GLU	CD-OE2	5.78	1.32	1.25
1	B	43	SER	CB-OG	5.72	1.49	1.42
1	A	106	GLU	CD-OE2	5.61	1.31	1.25
1	A	17	GLU	CD-OE2	5.61	1.31	1.25
1	B	278	GLU	CD-OE1	5.56	1.31	1.25
1	B	159	SER	C-N	-5.06	1.22	1.34

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	ARG	NE-CZ-NH1	17.15	128.87	120.30
1	B	319	ARG	NE-CZ-NH2	-15.55	112.53	120.30
1	B	11	ASP	CB-CG-OD1	11.18	128.36	118.30
1	A	46(A)	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	B	314	ASP	CB-CG-OD2	-10.59	108.77	118.30
1	A	315	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	A	149	ASP	CB-CG-OD1	-10.15	109.16	118.30
1	B	46(A)	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	B	11	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	B	149	ASP	CB-CG-OD2	-9.48	109.77	118.30
1	A	263	GLY	C-N-CA	-9.46	102.44	122.30
1	A	46(A)	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	B	273	ASP	CB-CG-OD2	-9.05	110.16	118.30
1	A	171	ASP	CB-CG-OD1	8.95	126.35	118.30
1	B	171	ASP	CB-CG-OD2	-8.93	110.26	118.30
1	B	157	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	B	32	ASP	CB-CG-OD1	8.58	126.02	118.30
1	B	171	ASP	CB-CG-OD1	8.52	125.97	118.30
1	A	11	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	A	158	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	A	244	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	171	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	315	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	A	215	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	B	273	ASP	CB-CG-OD1	7.85	125.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	B	208	ASP	CB-CG-OD1	7.74	125.27	118.30
1	B	157	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	A	208	ASP	N-CA-CB	7.61	124.30	110.60
1	A	244	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	314	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	A	11	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	71	LEU	CB-CA-C	-7.26	96.40	110.20
1	A	208	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	314	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	158	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	316	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	138	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	B	314	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	270	THR	N-CA-CB	-6.66	97.64	110.30
1	A	26	THR	N-CA-CB	-6.65	97.67	110.30
1	B	97	THR	CA-CB-CG2	-6.57	103.20	112.40
1	A	118	ASP	CB-CG-OD1	6.50	124.16	118.30
1	B	87	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	10	MET	CG-SD-CE	6.34	110.35	100.20
1	A	133	VAL	CG1-CB-CG2	-6.20	100.98	110.90
1	B	319	ARG	CD-NE-CZ	6.04	132.05	123.60
1	A	273	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	57	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	32	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	B	144	GLY	N-CA-C	-5.74	98.76	113.10
1	A	279	SER	N-CA-CB	5.71	119.06	110.50
1	A	307	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	326	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	189	VAL	CA-CB-CG1	5.66	119.39	110.90
1	B	257	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	87	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	323	ALA	N-CA-CB	5.57	117.90	110.10
1	A	257	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	120	VAL	CA-CB-CG1	5.44	119.06	110.90
1	B	150	VAL	CA-CB-CG1	5.44	119.05	110.90
1	B	145	VAL	CA-CB-CG1	5.40	119.00	110.90
1	B	279	SER	N-CA-CB	-5.40	102.41	110.50
1	B	149	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	87	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	244	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	B	95	THR	OG1-CB-CG2	5.30	122.19	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	283	THR	CA-CB-CG2	-5.21	105.11	112.40
1	B	278	GLU	CB-CA-C	-5.20	100.00	110.40
1	A	180	HIS	CA-CB-CG	-5.19	104.78	113.60
1	A	290	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	70	GLU	CA-CB-CG	-5.17	102.02	113.40
1	A	118	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	157	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	300	ALA	N-CA-CB	5.09	117.23	110.10
1	A	203	THR	N-CA-CB	5.08	119.95	110.30
1	B	199	VAL	CB-CA-C	5.02	120.94	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	95	THR	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	2576	0	2506	94	0
1	B	2551	0	2467	126	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	36	0	49	0	0
3	B	36	0	49	6	0
4	A	206	0	0	14	1
4	B	160	0	0	11	1
All	All	5593	0	5097	220	1

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 21.

All (220) 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:46(A):ARG:HG3	1:B:46(A):ARG:HH11	1.26	0.97
1:A:156:ASN:HD22	1:A:157:ARG:H	1.18	0.92
1:A:185:ILE:HG22	1:A:186:LYS:HG2	1.57	0.86
1:A:25:GLN:HE22	1:A:57:ASP:H	1.23	0.86
1:B:49:ALA:CB	1:B:107:MET:HG2	2.10	0.80
1:A:226:SER:HA	1:A:229:GLU:HG2	1.64	0.79
1:B:20:ILE:HG12	1:B:89:ILE:HG12	1.63	0.78
1:B:253:PRO:HB2	4:B:1160:HOH:O	1.84	0.77
1:B:47:TYR:OH	1:B:106:GLU:HG3	1.86	0.76
1:B:289:MET:HG2	3:B:391:03D:H16A	1.67	0.76
1:B:314:ASP:OD2	1:B:319:ARG:HD2	1.87	0.75
1:B:46(A):ARG:HG3	1:B:46(A):ARG:NH1	1.94	0.74
1:A:211:LEU:HB2	1:A:298:THR:HG23	1.68	0.74
1:B:41:PRO:HB2	1:B:55:LEU:HD23	1.70	0.74
1:B:71:LEU:HD11	1:B:84:LEU:HD13	1.69	0.73
1:B:8:ASN:HD21	1:B:11:ASP:H	1.36	0.73
1:A:289:MET:HB3	4:A:1094:HOH:O	1.89	0.72
1:A:156:ASN:HD22	1:A:157:ARG:N	1.87	0.71
1:A:8:ASN:HD21	1:A:11:ASP:H	1.37	0.71
1:A:283:THR:HG22	1:A:284:LEU:N	2.07	0.70
1:B:261:HIS:HB3	4:B:872:HOH:O	1.90	0.70
1:A:202:SER:OG	1:A:204:LEU:HD23	1.91	0.70
1:B:279(B):SER:HB2	1:B:279(D):LYS:H	1.57	0.69
1:B:64:TYR:OH	1:B:66:HIS:HA	1.93	0.68
1:B:51:VAL:HG12	1:B:52:TYR:CD1	2.29	0.68
1:B:51:VAL:HG12	1:B:52:TYR:CE1	2.29	0.67
1:A:252:GLY:HA3	1:A:277:GLN:HE22	1.58	0.67
1:B:160(D):SER:N	4:B:937:HOH:O	2.27	0.67
1:B:42:SER:O	1:B:55:LEU:HD22	1.94	0.67
3:B:391:03D:H25A	3:B:391:03D:H3	1.77	0.67
1:A:156:ASN:ND2	1:A:157:ARG:H	1.90	0.66
1:B:193:GLN:HG2	1:B:195:LYS:NZ	2.10	0.66
1:A:195:LYS:NZ	1:A:263:GLY:H	1.93	0.66
1:B:49:ALA:HB3	1:B:107:MET:HG2	1.78	0.65
1:A:326:ARG:NH1	4:A:1110:HOH:O	2.29	0.65
1:B:77:THR:HB	1:B:111:PRO:HG3	1.79	0.65
1:A:187:THR:OG1	1:A:318:ASN:ND2	2.29	0.65
1:B:225:THR:O	1:B:229:GLU:HG3	1.97	0.64
1:A:315:ARG:NH2	4:A:982:HOH:O	2.30	0.64
1:A:270:THR:HG21	4:B:956:HOH:O	1.96	0.64
1:B:64:TYR:CZ	1:B:66:HIS:HA	2.32	0.63
1:B:226:SER:O	1:B:230:LYS:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASN:ND2	1:B:11:ASP:H	1.95	0.63
1:B:193:GLN:HG2	1:B:195:LYS:HZ3	1.63	0.63
1:B:235:LEU:HD12	1:B:256:PRO:HD2	1.80	0.63
1:A:244:ASP:OD2	1:A:283:THR:HG23	2.00	0.62
1:A:226:SER:O	1:A:229:GLU:HG3	1.99	0.62
1:A:147:LYS:HD2	1:A:148:GLU:HG3	1.81	0.62
1:A:160(A):ASN:N	4:A:898:HOH:O	2.32	0.62
1:A:211:LEU:CB	1:A:298:THR:HG23	2.30	0.62
1:A:174:HIS:HE1	4:A:1005:HOH:O	1.83	0.62
1:B:213:LEU:HD11	3:B:391:03D:H35A	1.82	0.61
1:B:49:ALA:HB1	1:B:107:MET:HG2	1.83	0.61
1:A:271:SER:N	4:A:892:HOH:O	2.33	0.60
1:A:133:VAL:HG23	4:A:837:HOH:O	2.01	0.60
1:B:8:ASN:HD21	1:B:11:ASP:N	2.00	0.59
1:A:8:ASN:ND2	1:A:11:ASP:H	2.00	0.59
1:A:141:ILE:HD12	1:A:149:ASP:OD1	2.02	0.59
1:B:173:GLN:HA	1:B:326:ARG:HH21	1.67	0.58
1:A:8:ASN:HD21	1:A:11:ASP:N	2.01	0.57
1:A:314:ASP:OD2	1:A:319:ARG:HD2	2.04	0.57
1:B:283:THR:C	1:B:284:LEU:HD23	2.24	0.57
1:B:68:GLY:O	1:B:69:THR:C	2.39	0.57
1:B:82:GLY:HA3	1:B:103:GLU:O	2.04	0.57
1:B:140:ILE:O	1:B:143:GLN:HB3	2.05	0.57
1:A:156:ASN:ND2	1:A:157:ARG:N	2.50	0.57
1:A:270:THR:HG23	4:B:875:HOH:O	2.03	0.57
1:A:287:HIS:HE1	4:A:1096:HOH:O	1.87	0.57
1:A:185:ILE:CG2	1:A:186:LYS:HG2	2.34	0.56
1:B:111:PRO:HD2	1:B:112:PHE:CE2	2.39	0.56
1:B:183:ASN:HD22	1:B:319:ARG:HB3	1.70	0.56
1:A:283:THR:HG22	1:A:284:LEU:H	1.70	0.56
1:A:138:ASP:OD1	1:A:315:ARG:NH2	2.39	0.56
1:A:-1:ASN:O	1:A:-1:ASN:ND2	2.38	0.56
1:B:316:ARG:HB3	4:B:953:HOH:O	2.05	0.55
1:A:199:VAL:CG2	1:A:231:LEU:HD12	2.37	0.55
1:A:240:ARG:HD2	1:A:246:VAL:HG13	1.87	0.55
1:A:71:LEU:HD23	1:A:71:LEU:N	2.21	0.55
1:A:252:GLY:HA3	1:A:277:GLN:NE2	2.21	0.55
1:B:41:PRO:CB	1:B:55:LEU:HD23	2.36	0.54
1:A:46(A):ARG:HD2	4:A:874:HOH:O	2.07	0.54
1:A:277:GLN:HG2	4:A:969:HOH:O	2.07	0.54
1:A:185:ILE:HG22	1:A:186:LYS:CG	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:HG22	1:A:186:LYS:N	2.22	0.54
1:B:125:PHE:CE2	1:B:315:ARG:HD3	2.43	0.54
1:A:8:ASN:HD22	1:A:8:ASN:C	2.12	0.53
1:B:48:THR:HG22	4:B:1069:HOH:O	2.08	0.53
1:B:60:ASP:N	1:B:60:ASP:OD1	2.38	0.53
1:B:11:ASP:OD1	1:B:158:ASP:HB2	2.08	0.53
1:B:204:LEU:HD13	1:B:205:LEU:HG	1.91	0.53
1:B:51:VAL:CG1	1:B:52:TYR:CE1	2.92	0.53
1:B:161:LEU:HD23	1:B:161:LEU:O	2.08	0.53
1:B:8:ASN:C	1:B:8:ASN:HD22	2.12	0.53
1:B:195:LYS:HG3	4:B:1065:HOH:O	2.09	0.52
1:B:42:SER:O	1:B:55:LEU:HB3	2.08	0.52
1:B:86:GLN:OE1	1:B:97:THR:HG22	2.10	0.52
1:A:226:SER:HA	1:A:229:GLU:CG	2.39	0.51
1:B:73:LEU:O	1:B:79:THR:HA	2.10	0.51
1:B:42:SER:C	1:B:55:LEU:HB3	2.31	0.50
1:A:240:ARG:HD3	1:A:244:ASP:OD1	2.11	0.50
1:B:199:VAL:HG13	1:B:256:PRO:HG2	1.94	0.50
1:A:63:SER:CB	1:A:88:ILE:HD12	2.42	0.50
1:B:252:GLY:C	1:B:254:THR:H	2.16	0.50
1:A:315:ARG:O	1:A:316:ARG:C	2.49	0.50
1:A:43:SER:O	1:A:46(A):ARG:NH2	2.44	0.50
1:B:150:VAL:HG13	1:B:312:GLU:HG3	1.92	0.49
1:B:200:GLY:HA2	4:B:1164:HOH:O	2.11	0.49
1:B:289:MET:HG2	3:B:391:03D:C16	2.40	0.49
1:B:144:GLY:O	1:B:145:VAL:HB	2.11	0.49
1:B:205:LEU:HD21	1:B:230:LYS:HB2	1.93	0.49
1:B:161:LEU:HD23	1:B:161:LEU:N	2.27	0.49
1:A:84:LEU:HD13	1:A:100:MET:CE	2.43	0.49
1:A:8:ASN:HD21	1:A:11:ASP:HA	1.78	0.49
1:A:253:PRO:HD3	1:A:277:GLN:NE2	2.27	0.49
1:B:180:HIS:ND1	4:B:936:HOH:O	2.35	0.48
1:B:271:SER:HA	1:B:274:TYR:CE2	2.47	0.48
1:B:130:ILE:HD12	1:B:130:ILE:N	2.28	0.48
1:B:203:THR:HG22	1:B:207:GLU:OE1	2.13	0.48
1:A:90:THR:HA	1:A:94:ILE:O	2.13	0.48
1:B:39:TRP:NE1	1:B:120:VAL:HG13	2.29	0.48
1:B:199:VAL:CG1	1:B:256:PRO:HG2	2.44	0.47
1:B:180:HIS:HE1	1:B:263:GLY:O	1.96	0.47
1:A:248:LYS:HE3	1:A:251:GLU:HG3	1.95	0.47
1:A:63:SER:HB2	1:A:88:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ASN:HD22	1:B:157:ARG:H	1.63	0.47
1:A:133:VAL:HG23	1:A:133:VAL:O	2.15	0.47
1:B:252:GLY:HA3	1:B:277:GLN:HE22	1.80	0.46
1:B:198:SER:OG	1:B:261:HIS:HE1	1.98	0.46
1:B:-1:ASN:HA	1:B:147:LYS:HG3	1.97	0.46
1:B:10:MET:O	1:B:11:ASP:HB2	2.16	0.46
1:B:199:VAL:O	1:B:200:GLY:C	2.52	0.46
1:B:99:GLN:NE2	1:B:136:ILE:HA	2.30	0.46
1:B:107:MET:O	1:B:107:MET:HG2	2.16	0.46
1:B:130:ILE:CD1	1:B:130:ILE:N	2.79	0.46
1:A:248:LYS:O	1:A:251:GLU:HB2	2.16	0.46
1:B:233:GLU:HG3	1:B:233:GLU:O	2.14	0.46
1:A:148:GLU:O	1:A:168:GLY:HA2	2.16	0.45
1:B:261:HIS:ND1	1:B:261:HIS:N	2.64	0.45
1:A:195:LYS:HZ3	1:A:263:GLY:H	1.64	0.45
1:B:161:LEU:N	1:B:161:LEU:CD2	2.79	0.45
1:A:3:SER:HA	1:A:165:ILE:O	2.17	0.45
1:A:186:LYS:HB3	1:A:186:LYS:HE3	1.65	0.45
1:A:316:ARG:CZ	1:A:317:ASN:ND2	2.79	0.45
1:B:204:LEU:HB3	1:B:205:LEU:HG	1.99	0.45
1:B:97:THR:HG21	4:B:1016:HOH:O	2.17	0.45
1:A:84:LEU:HD13	1:A:100:MET:HE1	1.98	0.45
1:A:183:ASN:OD1	1:A:183:ASN:N	2.49	0.45
1:A:283:THR:CG2	1:A:284:LEU:N	2.78	0.45
1:B:279(B):SER:OG	1:B:280:LYS:HB2	2.17	0.45
1:A:278:GLU:O	1:A:279:SER:HB3	2.16	0.45
1:B:284:LEU:N	1:B:284:LEU:HD23	2.29	0.45
1:B:48:THR:O	1:B:52:TYR:N	2.49	0.44
1:A:276:PHE:CE2	1:A:285:ALA:HB2	2.52	0.44
1:B:111:PRO:HB2	3:B:391:03D:H8	1.99	0.44
1:B:181:TYR:CD2	1:B:319:ARG:HD3	2.51	0.44
1:A:8:ASN:HD21	1:A:11:ASP:CA	2.30	0.44
1:A:128:GLN:HG3	4:A:902:HOH:O	2.16	0.44
1:A:193:GLN:O	1:A:195:LYS:NZ	2.48	0.44
1:B:157:ARG:HG2	1:B:307:ARG:HD2	1.98	0.44
1:B:152:SER:O	1:B:165:ILE:HA	2.17	0.44
1:B:293:PRO:HA	1:B:294:PRO:C	2.36	0.44
1:B:21:GLY:O	1:B:24:PRO:HA	2.17	0.44
1:B:43:SER:HB3	1:B:57:ASP:HA	2.00	0.44
1:A:253:PRO:HD3	1:A:277:GLN:HE22	1.82	0.44
1:A:280:LYS:HA	1:A:280:LYS:HD3	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:TYR:HD1	4:A:859:HOH:O	2.00	0.43
1:B:46(A):ARG:HB3	1:B:51:VAL:HG22	2.00	0.43
1:A:326:ARG:HH12	1:B:1:THR:HG22	1.84	0.43
1:B:228:ILE:O	1:B:232:MET:HG2	2.18	0.43
1:A:74:ARG:HD3	4:A:1149:HOH:O	2.18	0.43
1:B:296:GLY:HA2	1:B:297:PRO:C	2.39	0.43
1:B:111:PRO:HB2	3:B:391:03D:C8	2.49	0.43
1:A:316:ARG:CZ	1:A:317:ASN:HD21	2.31	0.43
1:B:125:PHE:HB3	1:B:127:GLU:OE1	2.19	0.43
1:A:249:CYS:HB3	1:A:279:SER:O	2.19	0.43
1:B:69:THR:HB	1:B:84:LEU:HD23	2.00	0.43
1:B:49:ALA:HB1	1:B:107:MET:CG	2.48	0.43
1:B:52:TYR:N	1:B:52:TYR:CD1	2.86	0.42
1:A:100:MET:HE3	1:A:100:MET:HB3	1.86	0.42
1:B:240:ARG:N	1:B:244:ASP:O	2.49	0.42
1:B:82:GLY:HA2	1:B:105:THR:HB	2.01	0.42
1:B:111:PRO:HD2	1:B:112:PHE:CD2	2.55	0.42
1:A:8:ASN:ND2	1:A:8:ASN:C	2.73	0.42
1:B:80:VAL:HG13	1:B:104:VAL:CG1	2.50	0.42
1:B:198:SER:OG	1:B:261:HIS:CE1	2.73	0.42
1:B:172:PRO:HA	1:B:175:TYR:CE1	2.54	0.42
1:B:0:THR:O	1:B:146:LEU:HA	2.20	0.42
1:A:174:HIS:HD2	1:A:326:ARG:OXT	2.02	0.41
1:A:215:ASP:O	1:A:302:GLY:HA2	2.18	0.41
1:A:242:LEU:HA	1:A:242:LEU:HD12	1.80	0.41
1:B:64:TYR:CG	1:B:65:LYS:N	2.88	0.41
1:A:278:GLU:HG3	4:A:992:HOH:O	2.19	0.41
1:B:134:THR:HA	1:B:135:PRO:HD3	1.91	0.41
1:A:184:LEU:O	1:A:185:ILE:C	2.56	0.41
1:B:150:VAL:HG22	1:B:314:ASP:HA	2.02	0.41
1:A:8:ASN:HD22	1:A:9:TYR:N	2.18	0.41
1:B:89:ILE:HD12	1:B:99:GLN:HG2	2.03	0.41
1:B:156:ASN:ND2	1:B:157:ARG:H	2.19	0.41
1:B:9:TYR:CD2	1:B:116:GLU:HG3	2.56	0.41
1:B:48:THR:HG22	1:B:52:TYR:CE1	2.56	0.41
1:B:125:PHE:CE2	1:B:315:ARG:CD	3.04	0.41
1:B:165:ILE:HD13	1:B:165:ILE:HG21	1.89	0.41
1:B:5:ILE:HD12	1:B:5:ILE:HG23	1.92	0.41
1:A:141:ILE:HD12	1:A:141:ILE:HG23	1.82	0.41
1:B:252:GLY:O	1:B:254:THR:N	2.54	0.41
1:A:195:LYS:HZ2	1:A:263:GLY:H	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HA	1:A:324:LEU:HD23	1.83	0.41
1:A:204:LEU:HD12	1:A:205:LEU:HG	2.01	0.40
1:B:48:THR:O	1:B:51:VAL:N	2.54	0.40
1:A:202:SER:O	1:A:204:LEU:N	2.54	0.40
1:A:199:VAL:HG22	1:A:231:LEU:HD12	2.03	0.40
1:B:51:VAL:C	1:B:52:TYR:CD1	2.95	0.40
1:B:252:GLY:N	1:B:253:PRO:HD2	2.37	0.40
1:B:8:ASN:HD21	1:B:11:ASP:HA	1.86	0.40
1:B:198:SER:O	1:B:258:ILE:HA	2.21	0.40
1:A:239:LYS:HG3	1:A:245:TYR:CZ	2.57	0.40
1:B:46(A):ARG:HB3	1:B:51:VAL:CG2	2.52	0.40
1:A:96:VAL:HG11	1:A:140:ILE:HG13	2.04	0.40
1:B:248:LYS:HB3	1:B:250:ASN:OD1	2.20	0.40
1:B:194:MET:O	1:B:209:GLY:HA2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:927:HOH:O	4:B:917:HOH:O[6_456]	2.11	0.09

## 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	331/337 (98%)	315 (95%)	14 (4%)	2 (1%)	30	14
1	B	330/337 (98%)	315 (96%)	12 (4%)	3 (1%)	21	7
All	All	661/674 (98%)	630 (95%)	26 (4%)	5 (1%)	24	8

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	279	SER
1	A	203	THR
1	B	242	LEU
1	B	112	PHE
1	B	253	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	284/287 (99%)	244 (86%)	40 (14%)	4	1
1	B	280/287 (98%)	240 (86%)	40 (14%)	4	1
All	All	564/574 (98%)	484 (86%)	80 (14%)	4	1

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	5	ILE
1	A	8	ASN
1	A	17	GLU
1	A	26	THR
1	A	28	LYS
1	A	96	VAL
1	A	116	GLU
1	A	135	PRO
1	A	138	ASP
1	A	147	LYS
1	A	149	ASP
1	A	156	ASN
1	A	173	GLN
1	A	186	LYS
1	A	187	THR
1	A	195	LYS
1	A	198	SER
1	A	204	LEU

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Mol	Chain	Res	Type
1	A	207	GLU
1	A	208	ASP
1	A	227	SER
1	A	229	GLU
1	A	238	LYS
1	A	239	LYS
1	A	247	VAL
1	A	254	THR
1	A	255	LEU
1	A	259	SER
1	A	265	LYS
1	A	270	THR
1	A	271	SER
1	A	279(C)	SER
1	A	279(D)	LYS
1	A	298	THR
1	A	315	ARG
1	A	316	ARG
1	A	319	ARG
1	A	324	LEU
1	A	326	ARG
1	B	1	THR
1	B	8	ASN
1	B	42	SER
1	B	43	SER
1	B	46	SER
1	B	46(A)	ARG
1	B	46(B)	LEU
1	B	47	TYR
1	B	48	THR
1	B	55	LEU
1	B	59	SER
1	B	60	ASP
1	B	62	SER
1	B	65	LYS
1	B	73	LEU
1	B	84	LEU
1	B	86	GLN
1	B	95	THR
1	B	97	THR
1	B	105	THR
1	B	110	LEU

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Mol	Chain	Res	Type
1	B	126	ILE
1	B	133	VAL
1	B	141	ILE
1	B	145	VAL
1	B	156	ASN
1	B	161	LEU
1	B	189	VAL
1	B	204	LEU
1	B	207	GLU
1	B	213	LEU
1	B	226	SER
1	B	233	GLU
1	B	235	LEU
1	B	248	LYS
1	B	254	THR
1	B	261	HIS
1	B	265	LYS
1	B	279(D)	LYS
1	B	319	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	8	ASN
1	A	25	GLN
1	A	99	GLN
1	A	139	ASN
1	A	156	ASN
1	A	174	HIS
1	A	277	GLN
1	A	317	ASN
1	A	318	ASN
1	B	8	ASN
1	B	99	GLN
1	B	139	ASN
1	B	156	ASN
1	B	174	HIS
1	B	180	HIS
1	B	183	ASN
1	B	261	HIS
1	B	277	GLN

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Mol	Chain	Res	Type
1	B	287	HIS
1	B	318	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	367	1	14,14,15	0.95	1 (7%)	15,19,21	1.66	4 (26%)
3	03D	A	391	-	37,38,38	1.36	3 (8%)	37,51,51	1.07	3 (8%)
2	NAG	B	367	1	14,14,15	1.61	2 (14%)	15,19,21	1.88	5 (33%)
3	03D	B	391	-	37,38,38	1.46	4 (10%)	37,51,51	1.07	4 (10%)

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	367	1	-	0/6/23/26	0/1/1/1
3	03D	A	391	-	-	0/40/50/50	0/2/3/3
2	NAG	B	367	1	-	0/6/23/26	0/1/1/1
3	03D	B	391	-	-	0/40/50/50	0/2/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	391	03D	C28-C23	2.01	1.57	1.52
3	B	391	03D	C28-C23	2.16	1.58	1.52
3	B	391	03D	C3-C4	2.36	1.57	1.51
3	B	391	03D	C22-C21	2.39	1.56	1.53
2	A	367	NAG	C8-C7	2.45	1.55	1.50
2	B	367	NAG	C8-C7	3.02	1.56	1.50
3	B	391	03D	C18-C15	3.45	1.59	1.53
3	A	391	03D	C3-C4	3.54	1.60	1.51
2	B	367	NAG	C1-C2	3.56	1.57	1.52
3	A	391	03D	C22-C21	3.63	1.58	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	367	NAG	C6-C5-C4	-3.54	104.29	113.02
3	B	391	03D	O19-C12-C13	-3.47	117.61	122.12
2	B	367	NAG	C1-O5-C5	-3.14	108.27	112.25
2	B	367	NAG	C4-C3-C2	-3.08	106.44	111.23
2	A	367	NAG	O7-C7-C8	-3.01	116.53	122.06
2	B	367	NAG	C6-C5-C4	-3.00	105.62	113.02
2	A	367	NAG	C4-C3-C2	-2.93	106.68	111.23
3	A	391	03D	O10-C1-C2	-2.52	104.63	109.79
3	A	391	03D	C25-C24-C23	-2.51	108.18	112.22
3	B	391	03D	C20-C21-N29	-2.23	105.87	110.31
3	B	391	03D	O11-C2-C3	-2.19	105.93	109.73
3	B	391	03D	C13-C12-N29	2.00	119.47	116.30
2	B	367	NAG	C8-C7-N2	2.02	119.98	116.11
2	A	367	NAG	C8-C7-N2	2.78	121.42	116.11
3	A	391	03D	O36-C31-C32	2.87	114.79	109.22
2	B	367	NAG	O4-C4-C3	3.67	118.60	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	391	03D	6	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.