Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 02:50 PM EDT

PDB ID	:	2REN
Title	:	STRUCTURE OF RECOMBINANT HUMAN RENIN, A TARGET FOR CA RDIOVASCULAR-ACTIVE DRUGS, AT 2.5 ANGSTROMS RESOLUTION
Authors	:	Sielecki, A.R.; James, M.N.G.
Deposited on	:	1992-02-05
Resolution	:	2.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

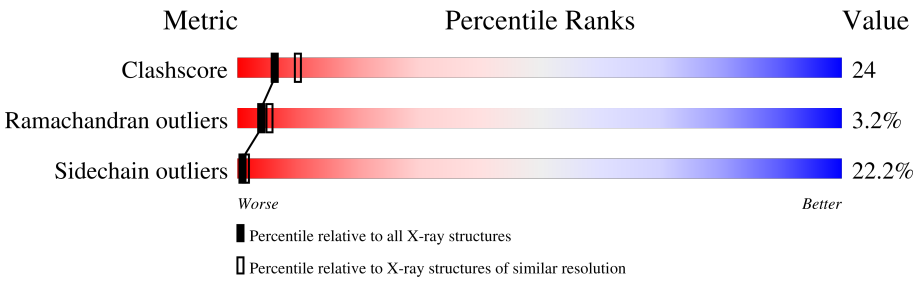
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	340	35% 38% 17% • 6%

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	341	X	-	-	-

2 Entry composition (i)

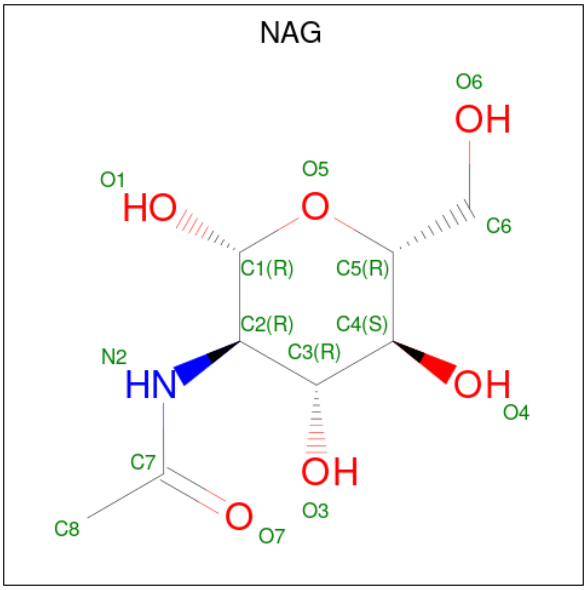
There are 2 unique types of molecules in this entry. The entry contains 2469 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	320	2455	1569	396	476	14	0	0	0

- 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

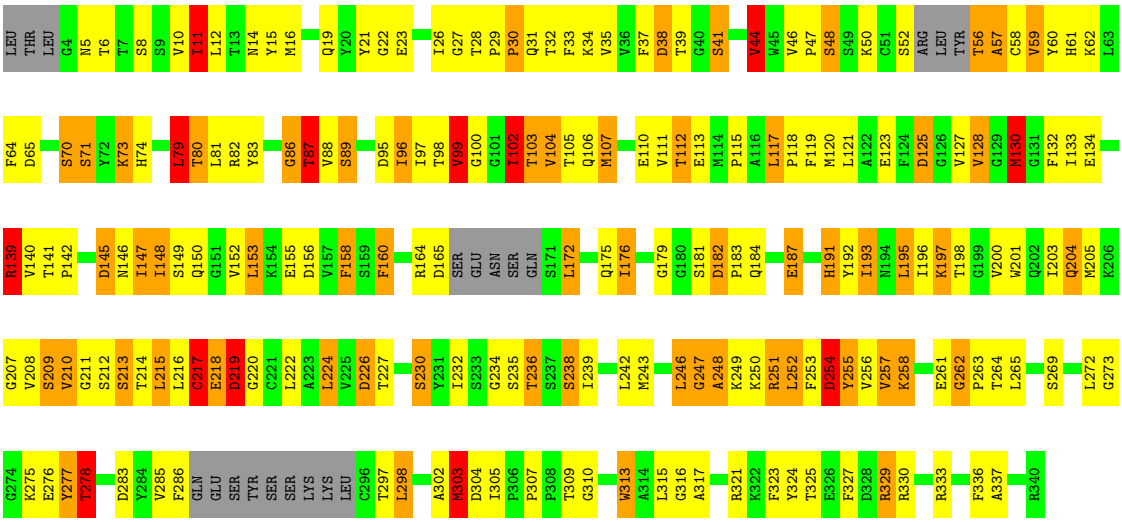
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: RENIN

Chain A: 35% 38% 17% • 6%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	134.08Å 134.08Å 41.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GROMOS, PROLSQ, X-PLOR	Depositor
R, R_{free}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2469	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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	0.94	0/2510	2.30	118/3402 (3.5%)

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	0	1

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	ARG	NE-CZ-NH2	-23.15	108.73	120.30
1	A	212	SER	N-CA-CB	14.20	131.80	110.50
1	A	182	ASP	CB-CG-OD2	12.54	129.58	118.30
1	A	253	PHE	C-N-CA	11.63	150.76	121.70
1	A	253	PHE	CA-C-O	11.54	144.33	120.10
1	A	172	LEU	CA-CB-CG	11.43	141.59	115.30
1	A	65	ASP	CB-CG-OD1	11.35	128.51	118.30
1	A	226	ASP	CB-CG-OD1	10.82	128.04	118.30
1	A	156	ASP	CB-CG-OD1	9.38	126.75	118.30
1	A	283	ASP	CB-CG-OD2	9.10	126.49	118.30
1	A	181	SER	N-CA-CB	9.00	124.00	110.50
1	A	198	THR	CA-CB-CG2	8.62	124.47	112.40
1	A	324	TYR	CB-CG-CD2	8.60	126.16	121.00
1	A	329	ARG	NH1-CZ-NH2	8.44	128.68	119.40
1	A	251	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	12	LEU	CA-CB-CG	8.28	134.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	LEU	CA-CB-CG	8.00	133.70	115.30
1	A	251	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	11	ILE	CB-CA-C	7.83	127.26	111.60
1	A	139	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	139	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	125	ASP	CB-CG-OD2	-7.52	111.54	118.30
1	A	182	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	A	329	ARG	CD-NE-CZ	7.38	133.94	123.60
1	A	251	ARG	CD-NE-CZ	7.34	133.87	123.60
1	A	203	ILE	CB-CA-C	7.32	126.25	111.60
1	A	324	TYR	CB-CG-CD1	-7.11	116.73	121.00
1	A	252	LEU	C-N-CA	7.00	139.19	121.70
1	A	164	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	191	HIS	N-CA-CB	6.90	123.02	110.60
1	A	298	LEU	CA-CB-CG	6.86	131.09	115.30
1	A	253	PHE	CA-CB-CG	-6.83	97.51	113.90
1	A	252	LEU	CA-C-O	6.82	134.43	120.10
1	A	52	SER	N-CA-CB	6.81	120.72	110.50
1	A	213	SER	N-CA-CB	-6.77	100.34	110.50
1	A	253	PHE	O-C-N	-6.76	111.89	122.70
1	A	37	PHE	CB-CA-C	6.72	123.85	110.40
1	A	86	GLY	CA-C-O	6.56	132.41	120.60
1	A	224	LEU	CA-CB-CG	6.56	130.39	115.30
1	A	58	CYS	CB-CA-C	6.52	123.44	110.40
1	A	46	VAL	CA-CB-CG1	6.48	120.62	110.90
1	A	44	VAL	CA-CB-CG1	6.43	120.55	110.90
1	A	6	THR	N-CA-C	6.31	128.03	111.00
1	A	307	PRO	N-CA-C	-6.31	95.70	112.10
1	A	321	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	A	156	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	107	MET	N-CA-C	-6.12	94.47	111.00
1	A	253	PHE	CA-C-N	-6.10	103.77	117.20
1	A	73	LYS	N-CA-CB	6.10	121.58	110.60
1	A	99	VAL	CB-CA-C	6.08	122.95	111.40
1	A	102	ILE	N-CA-C	-6.06	94.63	111.00
1	A	79	LEU	CA-CB-CG	6.05	129.21	115.30
1	A	191	HIS	N-CA-C	-6.01	94.77	111.00
1	A	38	ASP	N-CA-CB	-5.91	99.96	110.60
1	A	107	MET	CA-C-O	-5.90	107.71	120.10
1	A	112	THR	N-CA-CB	-5.89	99.11	110.30
1	A	103	THR	N-CA-C	-5.84	95.22	111.00
1	A	333	ARG	CD-NE-CZ	5.84	131.78	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	VAL	CA-CB-CG2	5.83	119.65	110.90
1	A	226	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	277	TYR	CA-CB-CG	-5.81	102.37	113.40
1	A	73	LYS	N-CA-C	-5.79	95.36	111.00
1	A	222	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	313	TRP	CA-CB-CG	5.78	124.68	113.70
1	A	337	ALA	N-CA-CB	5.78	118.19	110.10
1	A	283	ASP	OD1-CG-OD2	-5.76	112.35	123.30
1	A	323	PHE	CB-CG-CD2	-5.75	116.77	120.80
1	A	323	PHE	O-C-N	5.74	131.89	122.70
1	A	105	THR	CA-CB-CG2	-5.72	104.38	112.40
1	A	211	GLY	C-N-CA	5.68	135.89	121.70
1	A	160	PHE	CB-CA-C	-5.67	99.05	110.40
1	A	70	SER	CB-CA-C	-5.66	99.35	110.10
1	A	253	PHE	CB-CA-C	5.66	121.72	110.40
1	A	195	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	325	THR	CA-CB-OG1	-5.64	97.16	109.00
1	A	87	THR	N-CA-CB	5.58	120.90	110.30
1	A	79	LEU	CB-CA-C	5.54	120.74	110.20
1	A	31	GLN	O-C-N	5.54	131.56	122.70
1	A	254	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	A	146	ASN	N-CA-CB	-5.53	100.64	110.60
1	A	31	GLN	N-CA-C	-5.53	96.08	111.00
1	A	86	GLY	C-N-CA	5.51	135.47	121.70
1	A	30	PRO	N-CA-C	5.50	126.39	112.10
1	A	184	GLN	O-C-N	5.45	131.41	122.70
1	A	315	LEU	CB-CA-C	5.44	120.53	110.20
1	A	123	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	A	71	SER	N-CA-CB	-5.42	102.37	110.50
1	A	158	PHE	C-N-CA	5.40	135.20	121.70
1	A	50	LYS	N-CA-CB	5.37	120.27	110.60
1	A	254	ASP	CA-CB-CG	-5.37	101.60	113.40
1	A	21	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	A	16	MET	CA-CB-CG	5.33	122.37	113.30
1	A	6	THR	C-N-CA	5.33	135.02	121.70
1	A	70	SER	N-CA-CB	-5.32	102.52	110.50
1	A	232	ILE	CA-C-O	-5.32	108.93	120.10
1	A	262	GLY	N-CA-C	-5.31	99.82	113.10
1	A	218	GLU	N-CA-C	-5.31	96.67	111.00
1	A	121	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	A	46	VAL	CA-CB-CG2	-5.29	102.97	110.90
1	A	153	LEU	CA-CB-CG	5.23	127.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	ASN	CA-C-N	-5.21	105.73	117.20
1	A	148	ILE	CA-CB-CG1	5.21	120.90	111.00
1	A	187	GLU	OE1-CD-OE2	5.19	129.52	123.30
1	A	96	ILE	CB-CA-C	-5.18	101.25	111.60
1	A	5	ASN	O-C-N	5.17	130.97	122.70
1	A	278	THR	C-N-CA	5.15	134.58	121.70
1	A	217	CYS	CA-CB-SG	5.15	123.26	114.00
1	A	133	ILE	CA-CB-CG1	-5.14	101.23	111.00
1	A	113	GLU	N-CA-CB	5.12	119.82	110.60
1	A	6	THR	CA-CB-OG1	-5.10	98.30	109.00
1	A	130	MET	N-CA-CB	-5.06	101.49	110.60
1	A	329	ARG	CG-CD-NE	-5.05	101.20	111.80
1	A	28	THR	CA-CB-CG2	-5.04	105.34	112.40
1	A	128	VAL	CA-CB-CG2	5.04	118.45	110.90
1	A	59	VAL	CA-CB-CG2	5.02	118.43	110.90
1	A	191	HIS	O-C-N	5.02	130.74	122.70
1	A	38	ASP	N-CA-C	5.02	124.55	111.00
1	A	31	GLN	CB-CA-C	5.02	120.43	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2455	0	2381	119	0
2	A	14	0	13	0	0
All	All	2469	0	2394	119	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 24.

All (119) 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:243:MET:HG2	1:A:255:TYR:CD1	1.88	1.06
1:A:215:LEU:HD12	1:A:218:GLU:HG3	1.39	1.03
1:A:269:SER:OG	1:A:278:THR:HB	1.74	0.87
1:A:305:ILE:O	1:A:310:GLY:HA3	1.75	0.84
1:A:145:ASP:OD1	1:A:329:ARG:NH2	2.10	0.83
1:A:59:VAL:HB	1:A:60:TYR:CD1	2.14	0.82
1:A:80:THR:HG23	1:A:89:SER:HB3	1.62	0.81
1:A:8:SER:HB3	1:A:100:GLY:O	1.81	0.80
1:A:257:VAL:HG22	1:A:258:LYS:HD3	1.66	0.77
1:A:59:VAL:HB	1:A:60:TYR:HD1	1.46	0.77
1:A:196:ILE:HD12	1:A:204:GLN:HB2	1.68	0.76
1:A:303:MET:O	1:A:305:ILE:HG13	1.88	0.74
1:A:210:VAL:CG1	1:A:246:LEU:HD13	2.18	0.74
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.53	0.73
1:A:39:THR:HG21	1:A:327:PHE:CE2	2.24	0.73
1:A:104:VAL:HG21	1:A:147:ILE:HG22	1.71	0.71
1:A:27:GLY:HA2	1:A:95:ASP:OD1	1.90	0.70
1:A:10:VAL:HB	1:A:176:ILE:HG23	1.74	0.69
1:A:11:ILE:HD13	1:A:172:LEU:HD23	1.73	0.69
1:A:14:ASN:ND2	1:A:165:ASP:HB2	2.07	0.68
1:A:22:GLY:O	1:A:34:LYS:HA	1.94	0.68
1:A:249:LYS:HB2	1:A:256:VAL:O	1.94	0.66
1:A:56:THR:O	1:A:59:VAL:HG23	1.97	0.65
1:A:192:TYR:C	1:A:193:ILE:HD12	2.16	0.64
1:A:117:LEU:H	1:A:118:PRO:HD2	1.63	0.63
1:A:210:VAL:HG12	1:A:210:VAL:O	1.99	0.62
1:A:98:THR:HG23	1:A:103:THR:HG22	1.82	0.62
1:A:226:ASP:O	1:A:316:GLY:HA2	1.99	0.62
1:A:44:VAL:HB	1:A:128:VAL:HA	1.80	0.62
1:A:257:VAL:HG22	1:A:258:LYS:CD	2.31	0.60
1:A:152:VAL:HG23	1:A:153:LEU:HD12	1.83	0.59
1:A:88:VAL:HG13	1:A:111:VAL:CG1	2.33	0.59
1:A:236:THR:OG1	1:A:304:ASP:OD2	2.16	0.58
1:A:139:ARG:HG2	1:A:139:ARG:NH1	2.17	0.58
1:A:191:HIS:NE2	1:A:273:GLY:O	2.32	0.58
1:A:33:PHE:CZ	1:A:64:PHE:HB2	2.39	0.58
1:A:257:VAL:HG22	1:A:258:LYS:H	1.68	0.58
1:A:11:ILE:HD13	1:A:172:LEU:CD2	2.34	0.57
1:A:262:GLY:H	1:A:263:PRO:CD	2.17	0.57
1:A:87:THR:O	1:A:88:VAL:HG23	2.04	0.57
1:A:48:SER:HB2	1:A:110:GLU:OE2	2.06	0.56
1:A:57:ALA:HB2	1:A:120:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:HG22	1:A:99:VAL:HG12	1.88	0.56
1:A:44:VAL:HA	1:A:127:VAL:O	2.05	0.56
1:A:60:TYR:CD1	1:A:60:TYR:N	2.74	0.56
1:A:214:THR:O	1:A:215:LEU:CD2	2.55	0.55
1:A:258:LYS:HD3	1:A:258:LYS:H	1.72	0.54
1:A:262:GLY:H	1:A:263:PRO:HD2	1.71	0.54
1:A:261:GLU:HG2	1:A:264:THR:HG21	1.90	0.54
1:A:139:ARG:HH11	1:A:139:ARG:CG	2.20	0.54
1:A:15:TYR:HB3	1:A:19:GLN:HB2	1.91	0.53
1:A:209:SER:HA	1:A:214:THR:O	2.09	0.53
1:A:145:ASP:CG	1:A:329:ARG:HH22	2.13	0.52
1:A:88:VAL:HG13	1:A:111:VAL:HG13	1.92	0.51
1:A:305:ILE:C	1:A:310:GLY:HA3	2.31	0.51
1:A:257:VAL:CG2	1:A:258:LYS:HD3	2.39	0.51
1:A:26:ILE:HD12	1:A:33:PHE:CD1	2.46	0.51
1:A:269:SER:HG	1:A:278:THR:HB	1.76	0.50
1:A:47:PRO:HD3	1:A:125:ASP:O	2.12	0.50
1:A:234:GLY:O	1:A:302:ALA:HA	2.11	0.50
1:A:210:VAL:HG21	1:A:242:LEU:HG	1.94	0.49
1:A:39:THR:HG21	1:A:327:PHE:CZ	2.47	0.49
1:A:205:MET:CE	1:A:313:TRP:CD1	2.95	0.49
1:A:88:VAL:HG11	1:A:111:VAL:HG21	1.95	0.48
1:A:38:ASP:OD2	1:A:41:SER:HB3	2.13	0.48
1:A:61:HIS:HB3	1:A:125:ASP:OD1	2.13	0.48
1:A:196:ILE:CG2	1:A:197:LYS:HE2	2.43	0.48
1:A:215:LEU:HD12	1:A:218:GLU:CG	2.27	0.48
1:A:115:PRO:HD2	1:A:119:PHE:HD2	1.79	0.48
1:A:117:LEU:N	1:A:118:PRO:HD2	2.29	0.48
1:A:130:MET:HG2	1:A:158:PHE:CE2	2.49	0.47
1:A:215:LEU:CD1	1:A:218:GLU:HG3	2.27	0.47
1:A:235:SER:HB2	1:A:304:ASP:OD1	2.14	0.47
1:A:87:THR:O	1:A:115:PRO:HD3	2.14	0.47
1:A:285:VAL:HG22	1:A:298:LEU:HD12	1.95	0.47
1:A:71:SER:OG	1:A:95:ASP:OD1	2.32	0.47
1:A:258:LYS:CD	1:A:258:LYS:H	2.28	0.46
1:A:243:MET:CB	1:A:255:TYR:CE1	2.99	0.46
1:A:193:ILE:HD12	1:A:193:ILE:N	2.31	0.46
1:A:214:THR:O	1:A:215:LEU:HD23	2.15	0.46
1:A:193:ILE:N	1:A:193:ILE:CD1	2.79	0.46
1:A:214:THR:O	1:A:215:LEU:HD22	2.15	0.46
1:A:83:TYR:HB2	1:A:86:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:HA2	1:A:216:LEU:O	2.16	0.45
1:A:235:SER:OG	1:A:238:SER:HB2	2.17	0.45
1:A:33:PHE:HZ	1:A:64:PHE:HB2	1.82	0.44
1:A:243:MET:CG	1:A:255:TYR:CD1	2.80	0.44
1:A:38:ASP:HA	1:A:227:THR:OG1	2.17	0.44
1:A:254:ASP:O	1:A:255:TYR:O	2.35	0.44
1:A:160:PHE:CZ	1:A:227:THR:HG21	2.53	0.44
1:A:38:ASP:HA	1:A:227:THR:HG1	1.82	0.44
1:A:59:VAL:CB	1:A:60:TYR:CD1	2.94	0.43
1:A:196:ILE:HG23	1:A:197:LYS:HE2	2.00	0.43
1:A:132:PHE:HE1	1:A:201:TRP:CG	2.35	0.43
1:A:205:MET:O	1:A:220:GLY:HA2	2.18	0.43
1:A:23:GLU:HA	1:A:33:PHE:O	2.19	0.42
1:A:243:MET:HG2	1:A:255:TYR:HD1	1.66	0.42
1:A:303:MET:O	1:A:304:ASP:C	2.57	0.42
1:A:88:VAL:CG1	1:A:111:VAL:CG2	2.97	0.42
1:A:286:PHE:HB2	1:A:297:THR:O	2.20	0.42
1:A:97:ILE:O	1:A:103:THR:HA	2.19	0.42
1:A:132:PHE:HE1	1:A:201:TRP:CD2	2.37	0.42
1:A:182:ASP:HA	1:A:183:PRO:HD2	1.75	0.42
1:A:208:VAL:HB	1:A:216:LEU:HB2	2.02	0.42
1:A:239:ILE:HD11	1:A:313:TRP:CZ3	2.55	0.42
1:A:272:LEU:HD12	1:A:277:TYR:CD1	2.55	0.42
1:A:247:GLY:O	1:A:248:ALA:HB3	2.20	0.41
1:A:148:ILE:HD13	1:A:148:ILE:HG21	1.78	0.41
1:A:141:THR:HA	1:A:142:PRO:HD2	1.94	0.41
1:A:29:PRO:HA	1:A:30:PRO:HD3	1.90	0.41
1:A:155:GLU:O	1:A:179:GLY:HA2	2.21	0.41
1:A:230:SER:O	1:A:317:ALA:HB3	2.20	0.41
1:A:22:GLY:O	1:A:35:VAL:N	2.45	0.41
1:A:98:THR:HA	1:A:102:ILE:O	2.20	0.41
1:A:217:CYS:O	1:A:219:ASP:N	2.53	0.41
1:A:247:GLY:HA3	1:A:257:VAL:HG21	2.02	0.41
1:A:243:MET:HB3	1:A:255:TYR:CE1	2.55	0.40
1:A:88:VAL:HG13	1:A:111:VAL:HG11	2.02	0.40
1:A:79:LEU:O	1:A:89:SER:HA	2.20	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	312/340 (92%)	273 (88%)	29 (9%)	10 (3%)	4 5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	ASP
1	A	57	ALA
1	A	219	ASP
1	A	255	TYR
1	A	246	LEU
1	A	117	LEU
1	A	303	MET
1	A	248	ALA
1	A	247	GLY
1	A	210	VAL

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	270/290 (93%)	210 (78%)	60 (22%)	1 1

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE

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Mol	Chain	Res	Type
1	A	32	THR
1	A	41	SER
1	A	44	VAL
1	A	48	SER
1	A	56	THR
1	A	62	LYS
1	A	70	SER
1	A	73	LYS
1	A	74	HIS
1	A	79	LEU
1	A	80	THR
1	A	81	LEU
1	A	82	ARG
1	A	87	THR
1	A	89	SER
1	A	96	ILE
1	A	99	VAL
1	A	102	ILE
1	A	106	GLN
1	A	107	MET
1	A	112	THR
1	A	130	MET
1	A	134	GLU
1	A	139	ARG
1	A	140	VAL
1	A	145	ASP
1	A	147	ILE
1	A	149	SER
1	A	150	GLN
1	A	175	GLN
1	A	176	ILE
1	A	187	GLU
1	A	193	ILE
1	A	195	LEU
1	A	197	LYS
1	A	200	VAL
1	A	204	GLN
1	A	209	SER
1	A	213	SER
1	A	215	LEU
1	A	217	CYS
1	A	219	ASP

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	230	SER
1	A	236	THR
1	A	238	SER
1	A	250	LYS
1	A	251	ARG
1	A	252	LEU
1	A	254	ASP
1	A	257	VAL
1	A	258	LYS
1	A	265	LEU
1	A	275	LYS
1	A	276	GLU
1	A	278	THR
1	A	303	MET
1	A	309	THR
1	A	336	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS

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)

1 ligand is 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	341	1	14,14,15	1.53	2 (14%)	17,19,21	2.16	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	341	1	1/1/5/7	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	341	NAG	O5-C1	-3.89	1.37	1.43
2	A	341	NAG	C1-C2	-2.94	1.48	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	341	NAG	O5-C1-C2	5.32	119.52	111.29
2	A	341	NAG	C1-O5-C5	3.94	117.46	112.19
2	A	341	NAG	C2-N2-C7	-3.39	118.35	122.90
2	A	341	NAG	C4-C3-C2	-2.42	107.47	111.02
2	A	341	NAG	C3-C4-C5	-2.39	105.90	110.23
2	A	341	NAG	C1-C2-N2	2.05	113.66	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	341	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	341	NAG	O5-C5-C6-O6
2	A	341	NAG	C4-C5-C6-O6
2	A	341	NAG	O7-C7-N2-C2

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.