Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:50 AM GMT

PDB ID	:	2V11
Title	:	CRYSTAL STRUCTURE OF RENIN WITH INHIBITOR 6
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Deposited on	:	2007-05-21
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/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:

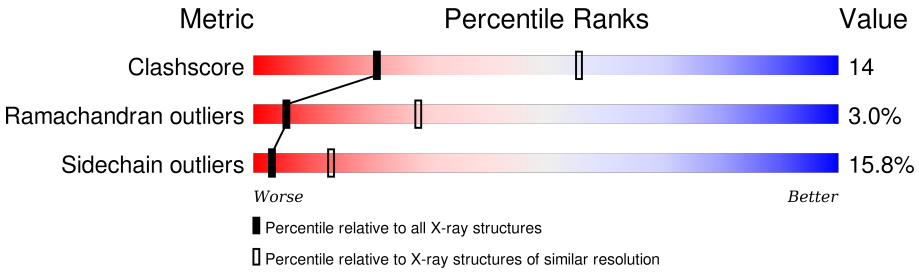
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	340	56% 31% 9%
1	O	340	50% 34% 10%

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	C80	C	1341	X	-	-	-
2	C80	O	1341	X	-	-	-

2 Entry composition

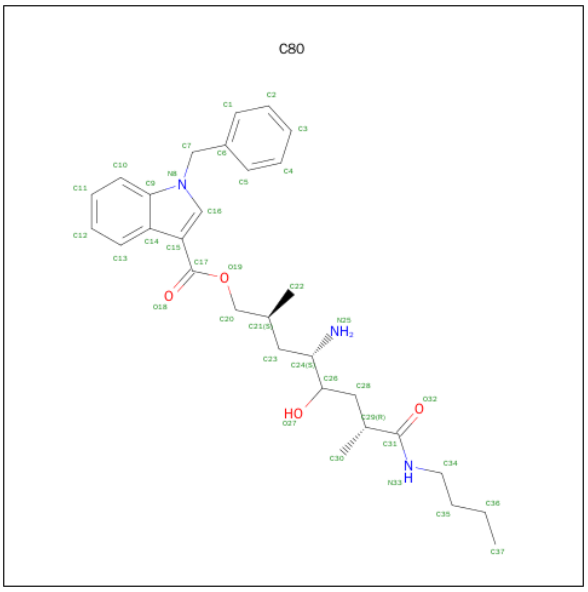
There are 2 unique types of molecules in this entry. The entry contains 5198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	C	334	Total	C	N	O	S	0	0	1
			2567	1639	416	498	14			
1	O	332	Total	C	N	O	S	0	0	1
			2557	1634	414	495	14			

- Molecule 2 is (2S,4S,5R,7R)-4-AMINO-8-(BUTYLAMINO)-5-HYDROXY-2,7-DIMETHYL-8-OXOOCTYL 1-BENZYL-1H-INDOLE-3-CARBOXYLATE (three-letter code: C80) (formula: $C_{30}H_{41}N_3O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			37	30	3	4		
2	O	1	Total	C	N	O	0	0
			37	30	3	4		

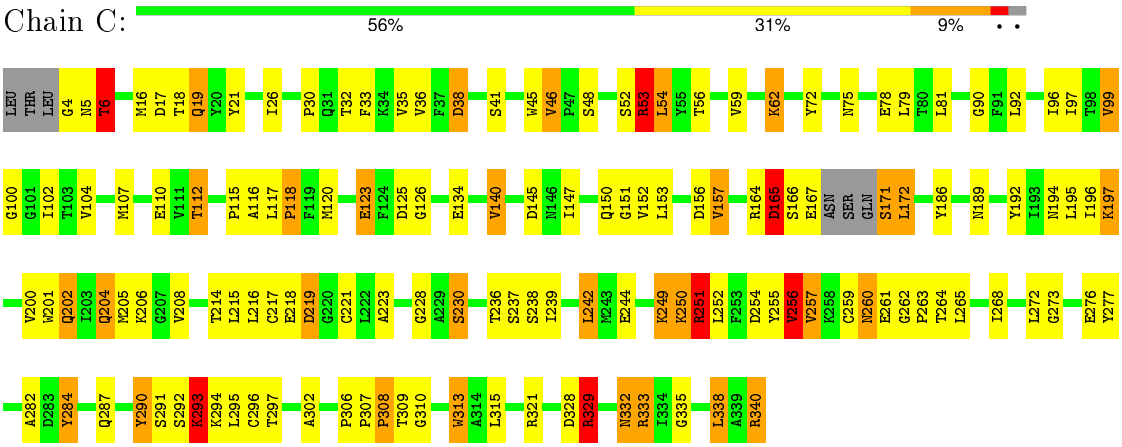
3 Residue-property plots (i)

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.

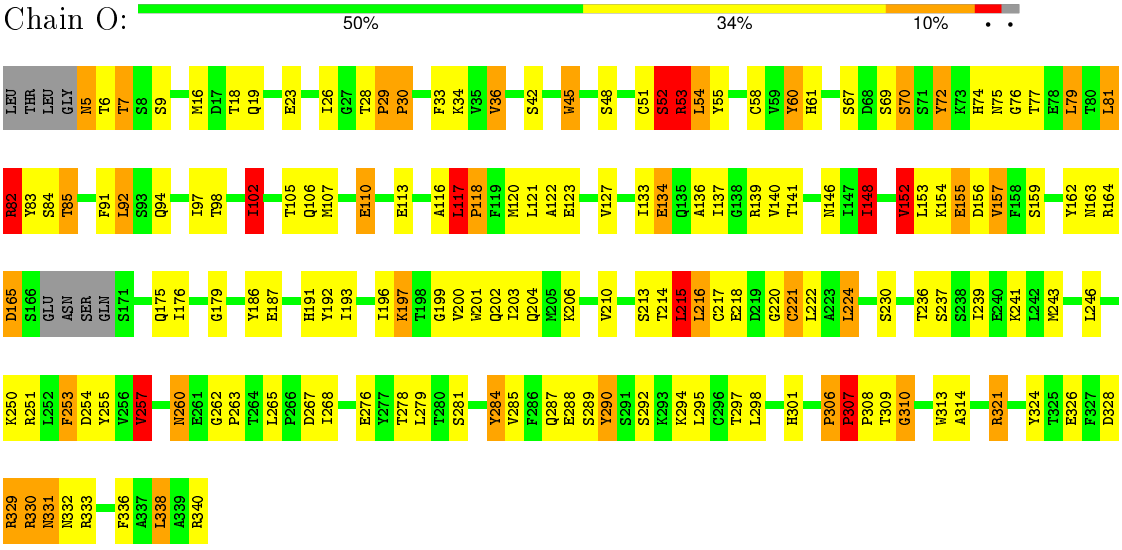
- Molecule 1: RENIN

Chain C:



- Molecule 1: RENIN

Chain O:



4 Data and refinement statistics (i)

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, α, β, γ	142.90Å 142.90Å 142.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	96.0 (10.00-3.10)	Depositor
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5198	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: C80

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	C	1.14	1/2626 (0.0%)	1.90	63/3560 (1.8%)
1	O	1.14	2/2616 (0.1%)	2.04	81/3547 (2.3%)
All	All	1.14	3/5242 (0.1%)	1.97	144/7107 (2.0%)

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	C	0	2
1	O	0	5
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	191	HIS	CB-CG	5.81	1.60	1.50
1	C	244	GLU	CG-CD	5.15	1.59	1.51
1	O	113	GLU	CB-CG	5.13	1.61	1.52

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	53	ARG	NE-CZ-NH2	-16.18	112.21	120.30
1	O	251	ARG	NE-CZ-NH2	-14.22	113.19	120.30
1	O	58	CYS	CA-CB-SG	-14.07	88.67	114.00
1	O	82	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	C	53	ARG	NE-CZ-NH1	12.83	126.71	120.30
1	O	53	ARG	NE-CZ-NH1	11.04	125.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	284	TYR	CB-CG-CD1	-9.67	115.20	121.00
1	C	204	GLN	CA-CB-CG	-9.33	92.88	113.40
1	C	6	THR	CA-CB-CG2	9.12	125.17	112.40
1	C	251	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	O	69	SER	CA-C-N	-8.64	98.19	117.20
1	O	321	ARG	NE-CZ-NH2	8.55	124.57	120.30
1	O	201	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	C	201	TRP	CG-CD2-CE3	8.25	141.33	133.90
1	C	244	GLU	CA-CB-CG	8.19	131.42	113.40
1	O	330	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	O	60	TYR	CB-CG-CD1	-8.00	116.20	121.00
1	O	313	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	O	329	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	C	45	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	C	75	ASN	CA-C-N	7.69	131.57	116.20
1	C	6	THR	CA-CB-OG1	-7.55	93.14	109.00
1	O	16	MET	CA-CB-CG	7.53	126.10	113.30
1	O	45	TRP	CB-CG-CD1	-7.53	117.22	127.00
1	O	313	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	O	257	VAL	CA-CB-CG1	-7.49	99.67	110.90
1	C	340	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	O	216	LEU	CB-CG-CD1	-7.37	98.47	111.00
1	O	201	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	C	290	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	C	293	LYS	CA-C-N	-7.32	101.11	117.20
1	O	83	TYR	CB-CG-CD1	-7.23	116.66	121.00
1	C	257	VAL	CA-CB-CG2	-7.22	100.07	110.90
1	O	162	TYR	CB-CG-CD2	-7.14	116.71	121.00
1	O	148	ILE	CA-CB-CG1	-7.11	97.50	111.00
1	C	36	VAL	CG1-CB-CG2	-7.08	99.58	110.90
1	C	112	THR	CA-CB-CG2	7.05	122.27	112.40
1	O	72	TYR	CB-CG-CD2	-7.05	116.77	121.00
1	O	253	PHE	N-CA-C	-6.92	92.33	111.00
1	O	45	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	O	313	TRP	CG-CD2-CE3	6.90	140.11	133.90
1	O	53	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	45	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	O	45	TRP	NE1-CE2-CZ2	-6.84	122.88	130.40
1	O	331	ASN	CA-C-N	-6.83	102.17	117.20
1	O	214	THR	CA-C-N	-6.79	102.26	117.20
1	O	82	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	C	282	ALA	N-CA-C	-6.75	92.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	102	ILE	CA-CB-CG2	-6.72	97.45	110.90
1	O	52	SER	N-CA-C	6.72	129.13	111.00
1	C	201	TRP	CB-CG-CD1	-6.63	118.38	127.00
1	O	251	ARG	CA-CB-CG	-6.60	98.87	113.40
1	O	329	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	313	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	O	45	TRP	CD1-CG-CD2	6.58	111.56	106.30
1	C	21	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	O	52	SER	N-CA-CB	-6.55	100.68	110.50
1	C	313	TRP	CG-CD2-CE3	6.52	139.77	133.90
1	C	313	TRP	CD1-CG-CD2	6.50	111.50	106.30
1	O	288	GLU	CA-C-N	-6.48	102.95	117.20
1	C	251	ARG	CB-CG-CD	6.47	128.42	111.60
1	C	5	ASN	O-C-N	6.42	132.98	122.70
1	C	201	TRP	CE2-CD2-CG	-6.35	102.22	107.30
1	C	201	TRP	CD1-CG-CD2	6.26	111.31	106.30
1	O	36	VAL	CA-CB-CG2	-6.19	101.61	110.90
1	C	242	LEU	CA-CB-CG	6.17	129.50	115.30
1	O	290	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	O	313	TRP	CB-CG-CD1	-6.14	119.02	127.00
1	C	172	LEU	CA-CB-CG	6.13	129.40	115.30
1	C	120	MET	CG-SD-CE	-6.11	90.43	100.20
1	O	214	THR	O-C-N	6.03	132.34	122.70
1	O	51	CYS	CA-CB-SG	-6.01	103.18	114.00
1	C	116	ALA	CB-CA-C	-5.99	101.11	110.10
1	O	215	LEU	CA-CB-CG	5.96	129.00	115.30
1	C	5	ASN	CA-C-N	-5.93	104.14	117.20
1	C	165	ASP	C-N-CA	5.92	136.51	121.70
1	C	276	GLU	CA-CB-CG	5.90	126.37	113.40
1	O	333	ARG	CG-CD-NE	-5.87	99.47	111.80
1	C	16	MET	CA-CB-CG	-5.84	103.37	113.30
1	C	164	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	O	45	TRP	CG-CD2-CE3	5.84	139.15	133.90
1	C	171	SER	CA-C-N	5.82	130.00	117.20
1	O	51	CYS	CA-C-N	-5.80	104.43	117.20
1	C	165	ASP	CA-C-N	-5.80	104.45	117.20
1	C	45	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	C	46	VAL	N-CA-CB	-5.74	98.88	111.50
1	O	79	LEU	CA-CB-CG	5.71	128.44	115.30
1	O	110	GLU	N-CA-C	-5.70	95.61	111.00
1	O	106	GLN	CA-CB-CG	5.69	125.91	113.40
1	O	52	SER	CA-C-N	5.68	129.69	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	145	ASP	CB-CG-OD1	5.64	123.38	118.30
1	O	5	ASN	CA-CB-CG	5.62	125.77	113.40
1	C	293	LYS	O-C-N	5.61	131.67	122.70
1	O	297	THR	CA-CB-CG2	5.59	120.23	112.40
1	O	105	THR	N-CA-C	-5.59	95.90	111.00
1	C	165	ASP	O-C-N	5.58	131.62	122.70
1	O	301	HIS	N-CA-CB	-5.56	100.59	110.60
1	O	276	GLU	CA-CB-CG	-5.56	101.17	113.40
1	C	112	THR	CA-CB-OG1	-5.53	97.39	109.00
1	O	201	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	C	125	ASP	CB-CG-OD1	5.50	123.25	118.30
1	O	33	PHE	CA-C-N	5.50	129.29	117.20
1	C	256	VAL	N-CA-CB	-5.48	99.43	111.50
1	C	249	LYS	CA-C-N	5.47	129.25	117.20
1	O	324	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	O	324	TYR	CA-C-N	5.47	129.24	117.20
1	C	45	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	C	140	VAL	CA-CB-CG2	-5.44	102.74	110.90
1	C	313	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	C	250	LYS	CA-C-N	5.43	129.14	117.20
1	C	46	VAL	CA-C-N	5.41	132.25	117.10
1	O	267	ASP	CB-CG-OD2	5.38	123.14	118.30
1	O	165	ASP	CA-CB-CG	5.35	125.17	113.40
1	C	251	ARG	CA-CB-CG	5.35	125.16	113.40
1	O	16	MET	N-CA-CB	-5.34	100.99	110.60
1	O	333	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	O	332	ASN	CB-CG-ND2	5.29	129.41	116.70
1	O	113	GLU	CB-CG-CD	5.26	128.40	114.20
1	C	201	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	C	30	PRO	CA-C-N	-5.25	105.65	117.20
1	O	81	LEU	CA-C-N	-5.23	105.69	117.20
1	C	208	VAL	N-CA-C	-5.22	96.91	111.00
1	C	284	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	C	340	ARG	N-CA-C	-5.20	96.97	111.00
1	O	152	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	O	221	CYS	CA-CB-SG	-5.15	104.73	114.00
1	C	329	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	O	60	TYR	CG-CD1-CE1	-5.12	117.20	121.30
1	O	201	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	O	121	LEU	O-C-N	-5.09	114.55	122.70
1	O	216	LEU	CA-C-N	-5.08	106.01	117.20
1	O	36	VAL	CA-CB-CG1	5.08	118.52	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	313	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	C	219	ASP	CA-CB-CG	-5.06	102.28	113.40
1	O	117	LEU	N-CA-C	-5.05	97.35	111.00
1	C	284	TYR	CA-CB-CG	5.05	122.99	113.40
1	O	257	VAL	CA-CB-CG2	5.04	118.47	110.90
1	O	7	THR	CA-CB-CG2	5.04	119.46	112.40
1	O	338	LEU	CB-CA-C	-5.04	100.63	110.20
1	O	157	VAL	CG1-CB-CG2	-5.02	102.87	110.90
1	C	208	VAL	CA-CB-CG2	-5.01	103.38	110.90
1	C	157	VAL	CB-CA-C	-5.01	101.88	111.40
1	O	34	LYS	CA-C-N	5.01	128.22	117.20
1	O	54	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	290	TYR	Sidechain
1	C	310	GLY	Peptide
1	O	186	TYR	Sidechain
1	O	29	PRO	Peptide
1	O	306	PRO	Peptide
1	O	307	PRO	Peptide
1	O	310	GLY	Peptide

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	C	2567	0	2498	68	0
1	O	2557	0	2490	79	0
2	C	37	0	40	4	0
2	O	37	0	40	2	0
All	All	5198	0	5068	147	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 14.

All (147) 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:C:19:GLN:HE21	1:C:123:GLU:H	1.19	0.89
1:O:48:SER:HB2	1:O:110:GLU:HB3	1.56	0.88
1:C:102:ILE:HG21	1:C:147:ILE:HG23	1.62	0.82
1:O:81:LEU:HD23	1:O:137:ILE:HD12	1.63	0.80
1:O:260:ASN:ND2	1:O:292:SER:HA	2.01	0.74
1:O:200:VAL:HG12	1:O:202:GLN:HB2	1.72	0.72
1:C:340:ARG:HH22	1:O:7:THR:HG22	1.54	0.71
1:O:5:ASN:N	1:O:154:LYS:HG3	2.05	0.71
1:O:52:SER:HG	1:O:55:TYR:HE1	1.36	0.71
1:O:5:ASN:CA	1:O:154:LYS:HG3	2.21	0.70
1:O:77:THR:HB	1:O:92:LEU:CD2	2.21	0.70
1:O:5:ASN:HA	1:O:154:LYS:HG3	1.74	0.69
1:O:196:ILE:HG23	1:O:197:LYS:HD3	1.74	0.69
1:O:246:LEU:HD11	1:O:268:ILE:HD11	1.76	0.68
1:O:210:VAL:HG12	1:O:268:ILE:HG12	1.76	0.68
1:C:157:VAL:HG12	1:C:328:ASP:HA	1.77	0.67
1:C:62:LYS:HB3	1:C:62:LYS:NZ	2.10	0.67
1:C:340:ARG:NH2	1:O:7:THR:HG22	2.09	0.67
1:C:261:GLU:O	1:C:264:THR:HB	1.94	0.66
1:O:257:VAL:HG21	1:O:265:LEU:HD11	1.76	0.66
1:C:260:ASN:OD1	1:C:292:SER:HA	1.94	0.65
1:C:48:SER:HB2	1:C:110:GLU:HB3	1.77	0.65
1:C:41:SER:HA	2:C:1341:C80:H373	1.79	0.65
1:O:79:LEU:HD12	1:O:92:LEU:HD22	1.80	0.64
1:O:77:THR:HB	1:O:92:LEU:HD21	1.79	0.64
1:O:26:ILE:HG12	1:O:97:ILE:HG12	1.81	0.62
1:O:213:SER:O	1:O:215:LEU:HB2	2.00	0.62
1:O:134:GLU:HG3	1:O:199:GLY:HA2	1.82	0.62
1:O:102:ILE:HG21	1:O:152:VAL:HG11	1.82	0.62
1:O:133:ILE:HD13	1:O:139:ARG:NE	2.15	0.61
1:O:187:GLU:HB3	1:O:338:LEU:HB2	1.82	0.61
1:O:60:TYR:CD1	1:O:120:MET:SD	2.93	0.60
1:O:196:ILE:HD12	1:O:204:GLN:HB2	1.84	0.60
1:C:56:THR:HA	1:C:59:VAL:HG12	1.83	0.60
1:C:150:GLN:HB3	1:C:152:VAL:HG13	1.83	0.59
1:O:133:ILE:HD13	1:O:139:ARG:HE	1.67	0.59
1:C:26:ILE:HG12	1:C:97:ILE:HG12	1.85	0.59
1:O:157:VAL:HG23	1:O:328:ASP:HA	1.85	0.59
1:C:200:VAL:HG12	1:C:202:GLN:HB2	1.86	0.58
1:C:19:GLN:HE21	1:C:123:GLU:N	1.97	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASP:OD1	1:C:329:ARG:HB2	2.04	0.57
1:C:265:LEU:HB3	1:C:284:TYR:OH	2.04	0.57
1:C:217:CYS:SG	1:C:221:CYS:N	2.78	0.57
1:O:134:GLU:HG3	1:O:199:GLY:CA	2.35	0.56
1:O:76:GLY:O	1:O:91:PHE:HB2	2.05	0.56
1:C:90:GLY:HA2	1:C:112:THR:HB	1.87	0.56
1:O:77:THR:HB	1:O:92:LEU:HD23	1.88	0.55
1:C:99:VAL:HG21	1:C:147:ILE:HD11	1.89	0.55
1:C:38:ASP:HB2	1:C:228:GLY:HA3	1.89	0.55
1:O:19:GLN:OE1	1:O:123:GLU:HB2	2.07	0.54
1:C:306:PRO:HG2	1:C:308:PRO:HG2	1.89	0.54
1:O:84:SER:O	1:O:85:THR:HG23	2.08	0.54
1:C:35:VAL:HA	1:C:126:GLY:O	2.09	0.53
1:C:195:LEU:HD22	1:C:332:ASN:HD22	1.73	0.53
1:C:107:MET:HB2	1:C:140:VAL:HG13	1.90	0.53
1:C:262:GLY:HA2	1:C:265:LEU:HD13	1.91	0.53
1:C:4:GLY:HA3	1:C:151:GLY:O	2.08	0.53
1:O:28:THR:HB	1:O:70:SER:HB2	1.90	0.52
1:C:194:ASN:HA	1:C:333:ARG:HB3	1.91	0.52
1:C:17:ASP:HB3	1:C:321:ARG:NH2	2.25	0.52
1:O:156:ASP:HB3	1:O:330:ARG:HB2	1.91	0.51
1:C:62:LYS:HZ3	1:C:62:LYS:HB3	1.76	0.51
1:O:60:TYR:HD1	1:O:120:MET:SD	2.33	0.51
1:C:38:ASP:OD2	1:C:41:SER:HB3	2.11	0.51
1:C:200:VAL:CG1	1:C:202:GLN:HB2	2.41	0.51
1:C:204:GLN:HG2	1:C:205:MET:N	2.25	0.50
1:O:217:CYS:SG	1:O:221:CYS:N	2.84	0.50
1:C:217:CYS:O	1:C:217:CYS:SG	2.70	0.50
1:O:156:ASP:O	1:O:329:ARG:HB2	2.12	0.50
1:O:243:MET:HG3	1:O:255:TYR:CD2	2.46	0.50
1:C:26:ILE:HD12	1:C:33:PHE:CD1	2.47	0.49
2:C:1341:C80:H16	2:C:1341:C80:H201	1.94	0.49
1:C:223:ALA:HA	1:C:313:TRP:O	2.12	0.49
1:O:215:LEU:HD11	1:O:241:LYS:HD2	1.92	0.49
1:C:262:GLY:N	1:C:263:PRO:HD2	2.26	0.49
1:C:307:PRO:HG2	1:C:308:PRO:HD2	1.94	0.49
1:C:251:ARG:HG3	1:C:254:ASP:OD2	2.13	0.49
1:C:167:GLU:N	1:C:171:SER:N	2.61	0.49
1:C:216:LEU:HD11	1:C:238:SER:O	2.12	0.49
1:C:6:THR:O	1:C:153:LEU:HA	2.13	0.49
1:O:260:ASN:H	1:O:260:ASN:HD22	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:213:SER:O	1:O:215:LEU:N	2.46	0.48
1:C:250:LYS:HG2	1:C:252:LEU:N	2.29	0.48
1:O:278:THR:O	1:O:279:LEU:HD23	2.13	0.48
1:O:6:THR:O	1:O:153:LEU:HA	2.13	0.48
1:O:60:TYR:CE1	1:O:120:MET:SD	3.07	0.48
1:C:196:ILE:HG23	1:C:197:LYS:HD2	1.94	0.48
1:O:75:ASN:HB3	1:O:92:LEU:O	2.14	0.47
1:C:239:ILE:HG13	1:C:302:ALA:HA	1.95	0.47
2:C:1341:C80:C16	2:C:1341:C80:H201	2.44	0.47
1:C:53:ARG:HD2	1:C:53:ARG:N	2.30	0.47
1:O:82:ARG:HG3	1:O:137:ILE:HD11	1.97	0.47
1:O:61:HIS:HE1	1:O:122:ALA:HB3	1.78	0.47
1:O:45:TRP:CD1	1:O:127:VAL:HG22	2.50	0.47
1:O:48:SER:HB2	1:O:110:GLU:CB	2.37	0.47
1:O:246:LEU:HD23	1:O:298:LEU:HD11	1.97	0.47
1:O:155:GLU:O	1:O:179:GLY:HA2	2.15	0.47
1:C:272:LEU:HB2	1:C:277:TYR:CE1	2.50	0.47
1:C:249:LYS:O	1:C:255:TYR:HA	2.15	0.47
1:O:217:CYS:SG	1:O:217:CYS:O	2.73	0.46
1:C:259:CYS:SG	1:C:296:CYS:N	2.88	0.46
1:C:308:PRO:HB2	1:C:309:THR:HG23	1.97	0.46
1:O:42:SER:HB2	1:O:136:ALA:HA	1.97	0.46
1:O:307:PRO:HA	1:O:310:GLY:H	1.81	0.46
1:C:18:THR:HA	1:C:230:SER:HB3	1.97	0.46
1:C:79:LEU:HD22	1:C:92:LEU:HD21	1.98	0.46
1:O:281:SER:HA	1:O:284:TYR:CE2	2.50	0.45
1:O:193:ILE:HG21	1:O:203:ILE:HD12	1.98	0.45
1:O:81:LEU:HA	1:O:137:ILE:HD12	1.97	0.45
1:C:19:GLN:NE2	1:C:123:GLU:H	1.99	0.45
1:C:196:ILE:CG2	1:C:197:LYS:HD2	2.47	0.45
1:O:53:ARG:HH11	1:O:53:ARG:HB3	1.80	0.45
1:C:256:VAL:HG11	1:C:295:LEU:HD13	1.99	0.45
1:O:192:TYR:N	1:O:192:TYR:CD1	2.85	0.44
1:O:200:VAL:CG1	1:O:202:GLN:HB2	2.43	0.44
1:O:92:LEU:HD12	1:O:107:MET:HG2	1.99	0.44
1:C:117:LEU:HA	1:C:118:PRO:HA	1.71	0.44
1:C:53:ARG:HD2	1:C:54:LEU:N	2.32	0.44
1:O:224:LEU:O	1:O:314:ALA:HA	2.16	0.44
1:C:250:LYS:HG2	1:C:252:LEU:H	1.83	0.44
1:C:260:ASN:N	1:C:291:SER:O	2.50	0.43
1:O:36:VAL:CG2	2:O:1341:C80:H4	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:116:ALA:O	1:O:120:MET:HB2	2.19	0.43
1:C:96:ILE:HD13	1:C:96:ILE:HG21	1.79	0.43
1:O:75:ASN:OD1	1:O:76:GLY:N	2.52	0.43
1:O:77:THR:O	1:O:91:PHE:HA	2.19	0.43
1:O:193:ILE:HD13	1:O:336:PHE:HD1	1.84	0.42
1:O:285:VAL:HG22	1:O:298:LEU:HD22	2.00	0.42
1:O:176:ILE:HD13	1:O:176:ILE:HG21	1.78	0.42
1:O:262:GLY:HA3	1:O:287:GLN:OE1	2.18	0.42
1:O:117:LEU:HA	1:O:118:PRO:HA	1.83	0.42
1:C:192:TYR:HA	1:C:335:GLY:HA2	2.00	0.41
1:O:52:SER:O	1:O:54:LEU:N	2.52	0.41
1:C:186:TYR:HA	1:C:338:LEU:O	2.20	0.41
1:O:148:ILE:HD12	1:O:148:ILE:HA	1.62	0.41
1:O:321:ARG:HH11	1:O:321:ARG:HD2	1.70	0.41
1:C:215:LEU:O	1:C:216:LEU:HD23	2.20	0.41
1:C:194:ASN:HA	1:C:333:ARG:CB	2.50	0.41
1:C:272:LEU:HB2	1:C:277:TYR:CD1	2.56	0.41
1:O:139:ARG:HA	1:O:139:ARG:HD2	1.75	0.41
1:C:292:SER:O	1:C:293:LYS:HG2	2.21	0.41
1:O:159:SER:HB3	1:O:326:GLU:HA	2.02	0.41
1:O:36:VAL:HG21	2:O:1341:C80:C4	2.51	0.41
1:O:72:TYR:CZ	1:O:74:HIS:HA	2.55	0.41
1:C:272:LEU:HD11	1:C:315:LEU:HD11	2.02	0.40
1:C:230:SER:N	2:C:1341:C80:H5	2.35	0.40
1:O:196:ILE:HG23	1:O:197:LYS:CD	2.44	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	C	330/340 (97%)	298 (90%)	25 (8%)	7 (2%)	9 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	O	328/340 (96%)	281 (86%)	34 (10%)	13 (4%)	4 21
All	All	658/680 (97%)	579 (88%)	59 (9%)	20 (3%)	5 28

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	214	THR
1	C	308	PRO
1	O	52	SER
1	O	85	THR
1	O	220	GLY
1	O	308	PRO
1	C	6	THR
1	C	166	SER
1	C	273	GLY
1	O	53	ARG
1	O	155	GLU
1	O	254	ASP
1	O	309	THR
1	C	100	GLY
1	C	165	ASP
1	O	30	PRO
1	O	70	SER
1	O	289	SER
1	O	263	PRO
1	O	307	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	C	283/290 (98%)	240 (85%)	43 (15%)	3 14
1	O	282/290 (97%)	236 (84%)	46 (16%)	3 12
All	All	565/580 (97%)	476 (84%)	89 (16%)	3 13

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	THR
1	C	19	GLN
1	C	32	THR
1	C	38	ASP
1	C	46	VAL
1	C	52	SER
1	C	53	ARG
1	C	54	LEU
1	C	62	LYS
1	C	72	TYR
1	C	78	GLU
1	C	81	LEU
1	C	99	VAL
1	C	104	VAL
1	C	115	PRO
1	C	118	PRO
1	C	123	GLU
1	C	134	GLU
1	C	165	ASP
1	C	172	LEU
1	C	189	ASN
1	C	197	LYS
1	C	202	GLN
1	C	206	LYS
1	C	218	GLU
1	C	219	ASP
1	C	230	SER
1	C	236	THR
1	C	237	SER
1	C	242	LEU
1	C	251	ARG
1	C	256	VAL
1	C	257	VAL
1	C	260	ASN
1	C	268	ILE
1	C	287	GLN
1	C	293	LYS
1	C	294	LYS
1	C	297	THR
1	C	329	ARG
1	C	332	ASN
1	C	333	ARG

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Mol	Chain	Res	Type
1	C	338	LEU
1	O	9	SER
1	O	18	THR
1	O	23	GLU
1	O	29	PRO
1	O	30	PRO
1	O	52	SER
1	O	53	ARG
1	O	67	SER
1	O	82	ARG
1	O	92	LEU
1	O	94	GLN
1	O	98	THR
1	O	102	ILE
1	O	117	LEU
1	O	118	PRO
1	O	134	GLU
1	O	140	VAL
1	O	141	THR
1	O	146	ASN
1	O	148	ILE
1	O	152	VAL
1	O	163	ASN
1	O	164	ARG
1	O	165	ASP
1	O	175	GLN
1	O	197	LYS
1	O	206	LYS
1	O	215	LEU
1	O	216	LEU
1	O	218	GLU
1	O	222	LEU
1	O	224	LEU
1	O	230	SER
1	O	236	THR
1	O	237	SER
1	O	239	ILE
1	O	250	LYS
1	O	253	PHE
1	O	257	VAL
1	O	260	ASN
1	O	290	TYR

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Mol	Chain	Res	Type
1	O	294	LYS
1	O	295	LEU
1	O	306	PRO
1	O	331	ASN
1	O	340	ARG

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

Mol	Chain	Res	Type
1	C	19	GLN
1	C	74	HIS
1	C	94	GLN
1	C	191	HIS
1	C	332	ASN
1	O	146	ASN
1	O	163	ASN
1	O	175	GLN
1	O	202	GLN
1	O	260	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	C80	C	1341	-	37,39,39	2.06	6 (16%)	39,52,52	2.61	11 (28%)
2	C80	O	1341	-	37,39,39	2.47	6 (16%)	39,52,52	2.55	11 (28%)

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	C80	C	1341	-	1/1/6/7	0/34/34/34	0/3/3/3
2	C80	O	1341	-	1/1/6/7	0/34/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1341	C80	C26-C24	-8.59	1.44	1.53
2	O	1341	C80	C15-C14	-7.41	1.36	1.42
2	C	1341	C80	C15-C14	-6.52	1.37	1.42
2	C	1341	C80	C26-C24	-5.70	1.47	1.53
2	O	1341	C80	C16-N8	-5.61	1.29	1.38
2	O	1341	C80	C15-C17	-4.96	1.40	1.50
2	C	1341	C80	C16-N8	-4.66	1.31	1.38
2	C	1341	C80	C15-C17	-4.50	1.41	1.50
2	O	1341	C80	O19-C17	-3.80	1.24	1.33
2	C	1341	C80	O19-C17	-3.36	1.25	1.33
2	O	1341	C80	C9-N8	-2.53	1.36	1.39
2	C	1341	C80	C9-N8	-2.29	1.36	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1341	C80	C20-O19-C17	-4.63	108.38	116.47
2	C	1341	C80	C22-C21-C20	-3.22	98.19	110.01
2	C	1341	C80	O19-C17-O18	-3.17	117.84	123.66
2	C	1341	C80	O32-C31-N33	-2.81	117.44	123.08
2	O	1341	C80	O19-C17-O18	-2.74	118.63	123.66
2	C	1341	C80	C15-C16-N8	-2.24	103.79	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1341	C80	C15-C16-N8	-2.19	103.89	108.60
2	C	1341	C80	C12-C13-C14	-2.17	117.81	120.88
2	O	1341	C80	C29-C31-N33	-2.05	113.95	116.84
2	C	1341	C80	C6-C7-N8	2.45	117.02	112.72
2	C	1341	C80	C16-C15-C14	2.51	115.05	108.09
2	O	1341	C80	C3-C4-C5	2.52	123.88	120.19
2	O	1341	C80	C16-C15-C14	2.65	115.44	108.09
2	O	1341	C80	C13-C14-C15	3.00	140.20	135.73
2	C	1341	C80	C29-C31-N33	4.00	122.51	116.84
2	O	1341	C80	C29-C28-C26	4.75	120.15	114.24
2	O	1341	C80	O19-C17-C15	4.79	121.00	111.87
2	O	1341	C80	C6-C7-N8	5.61	122.57	112.72
2	C	1341	C80	C29-C28-C26	6.08	121.80	114.24
2	C	1341	C80	O19-C17-C15	6.64	124.53	111.87
2	C	1341	C80	O27-C26-C28	9.78	128.17	109.22
2	O	1341	C80	O27-C26-C28	9.78	128.18	109.22

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1341	C80	C26
2	O	1341	C80	C26

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1341	C80	4	0
2	O	1341	C80	2	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.