



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2017 – 08:36 PM EDT

PDB ID : 2V10  
Title : Crystal Structure of Renin with Inhibitor 9  
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Deposited on : unknown  
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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

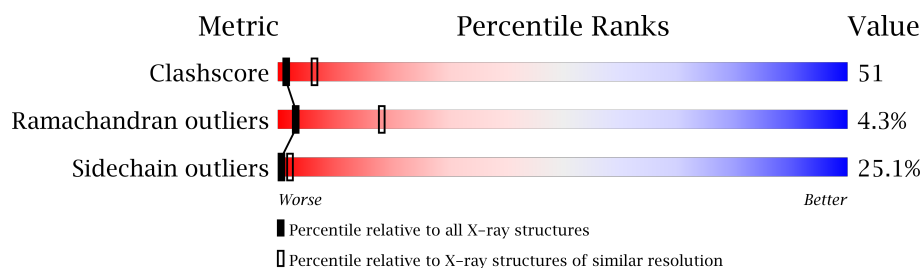
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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	C	340	
1	O	340	

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	C61	C	1341	-	-	X	-

## 2 Entry composition [i](#)

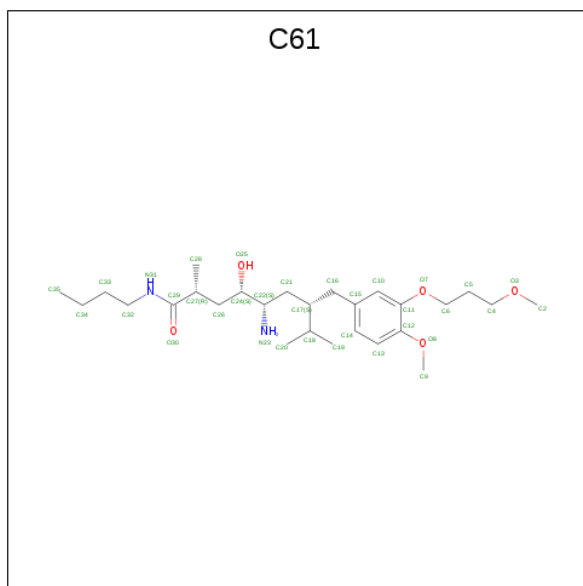
There are 2 unique types of molecules in this entry. The entry contains 5192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (2R,4S,5S,7S)-5-AMINO-N-BUTYL-4-HYDROXY-7-[4-METHOXY-3-(3-METHOXYPROPOXY)BENZYL]-2,8-DIMETHYLNONANAMIDE (three-letter code: C61) (formula: C<sub>27</sub>H<sub>48</sub>N<sub>2</sub>O<sub>5</sub>).



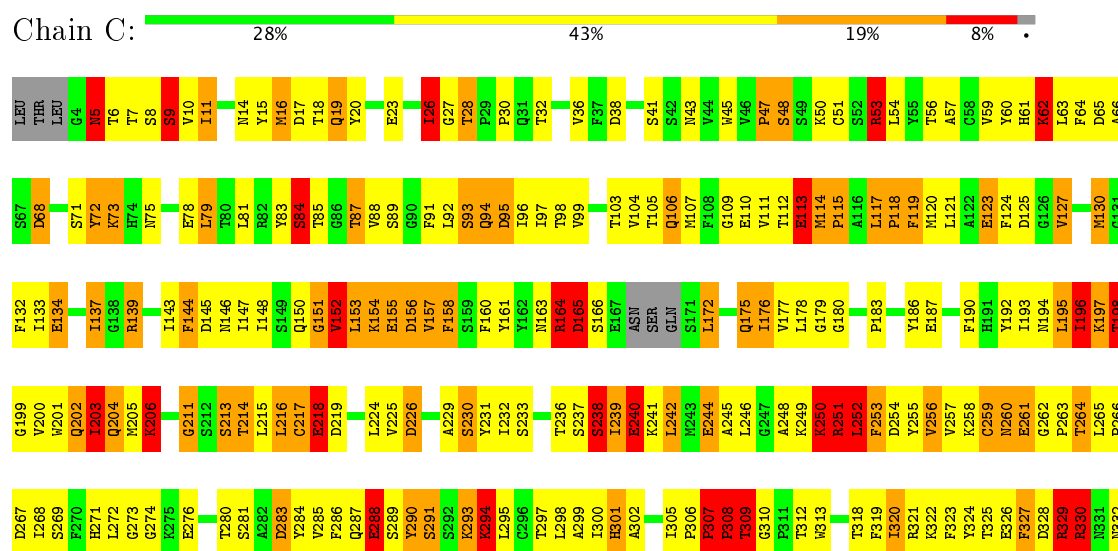
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			34	27	2	5		
2	O	1	Total	C	N	O	0	0
			34	27	2	5		

### 3 Residue-property plots

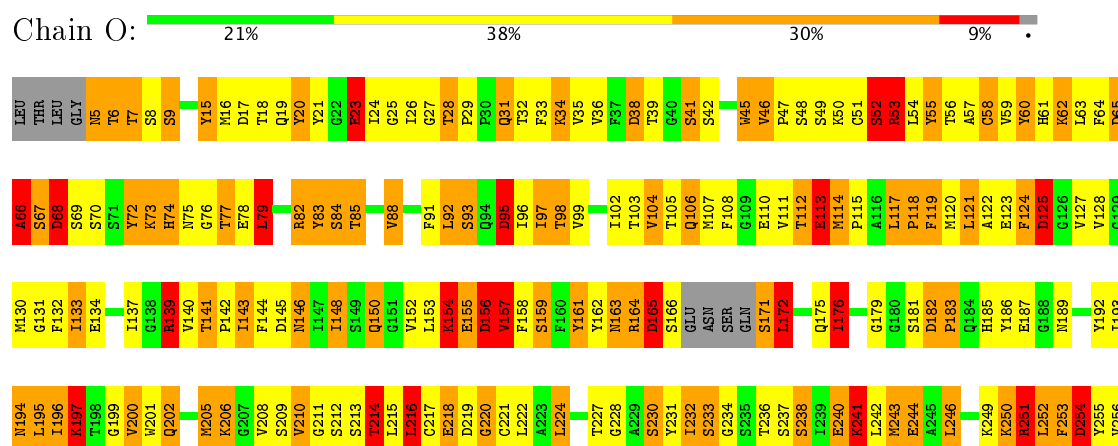
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

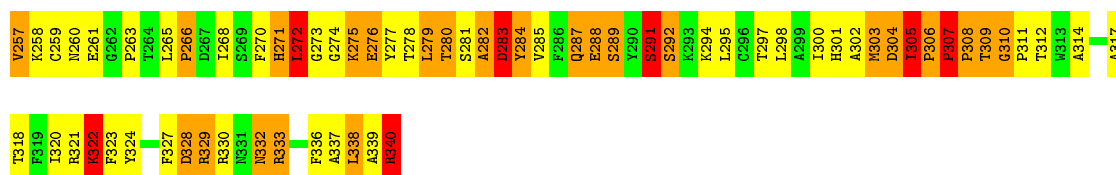
Note EDS was not executed.

#### • Molecule 1: RENIN



#### • Molecule 1: RENIN





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.00 Å   143.00 Å   143.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.10)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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: C61

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	1.62	31/2626 (1.2%)	2.25	133/3560 (3.7%)
1	O	1.59	24/2616 (0.9%)	2.41	169/3547 (4.8%)
All	All	1.60	55/5242 (1.0%)	2.33	302/7107 (4.2%)

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	5	0
1	O	3	0
All	All	8	0

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	ARG	NE-CZ	11.26	1.47	1.33
1	C	244	GLU	CD-OE2	11.00	1.37	1.25
1	O	288	GLU	CD-OE2	10.50	1.37	1.25
1	O	78	GLU	CD-OE2	9.96	1.36	1.25
1	C	218	GLU	CD-OE2	9.77	1.36	1.25
1	O	218	GLU	CD-OE2	9.36	1.35	1.25
1	C	288	GLU	CG-CD	9.33	1.66	1.51
1	O	113	GLU	CD-OE2	9.06	1.35	1.25
1	C	78	GLU	CD-OE2	9.05	1.35	1.25
1	O	123	GLU	CD-OE2	8.98	1.35	1.25
1	O	82	ARG	NE-CZ	8.93	1.44	1.33
1	O	276	GLU	CD-OE2	8.83	1.35	1.25
1	O	244	GLU	CD-OE2	8.72	1.35	1.25
1	O	261	GLU	CD-OE2	8.64	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	288	GLU	CD-OE2	8.35	1.34	1.25
1	O	240	GLU	CD-OE2	7.85	1.34	1.25
1	O	187	GLU	CD-OE2	7.52	1.33	1.25
1	O	253	PHE	CB-CG	7.51	1.64	1.51
1	C	240	GLU	CD-OE2	7.49	1.33	1.25
1	O	110	GLU	CD-OE2	7.37	1.33	1.25
1	C	110	GLU	CD-OE2	7.33	1.33	1.25
1	C	127	VAL	CB-CG2	-7.28	1.37	1.52
1	C	261	GLU	CD-OE2	7.18	1.33	1.25
1	C	123	GLU	CD-OE2	7.12	1.33	1.25
1	C	155	GLU	CD-OE2	6.99	1.33	1.25
1	O	164	ARG	NE-CZ	6.93	1.42	1.33
1	C	164	ARG	NE-CZ	6.85	1.42	1.33
1	O	139	ARG	NE-CZ	6.81	1.41	1.33
1	C	187	GLU	CD-OE1	-6.67	1.18	1.25
1	O	53	ARG	NE-CZ	6.55	1.41	1.33
1	C	113	GLU	CD-OE2	6.52	1.32	1.25
1	C	326	GLU	CD-OE2	6.44	1.32	1.25
1	O	155	GLU	CD-OE2	6.03	1.32	1.25
1	O	134	GLU	CD-OE2	6.00	1.32	1.25
1	C	276	GLU	CD-OE2	5.92	1.32	1.25
1	O	182	ASP	C-N	-5.82	1.23	1.34
1	C	164	ARG	CZ-NH2	5.74	1.40	1.33
1	O	276	GLU	CB-CG	5.68	1.62	1.52
1	C	288	GLU	CB-CG	5.67	1.62	1.52
1	O	119	PHE	N-CA	5.55	1.57	1.46
1	C	308	PRO	N-CA	-5.54	1.37	1.47
1	C	134	GLU	CD-OE2	5.42	1.31	1.25
1	C	251	ARG	CZ-NH2	5.39	1.40	1.33
1	C	251	ARG	CD-NE	5.33	1.55	1.46
1	C	72	TYR	CB-CG	-5.29	1.43	1.51
1	O	330	ARG	NE-CZ	5.26	1.39	1.33
1	O	183	PRO	CA-C	-5.25	1.42	1.52
1	C	72	TYR	C-N	-5.25	1.22	1.34
1	C	156	ASP	CA-C	-5.24	1.39	1.52
1	C	251	ARG	CZ-NH1	5.20	1.39	1.33
1	C	118	PRO	N-CA	-5.18	1.38	1.47
1	C	308	PRO	N-CD	5.16	1.55	1.47
1	O	58	CYS	CB-SG	-5.12	1.73	1.81
1	C	180	GLY	CA-C	5.12	1.60	1.51
1	C	23	GLU	CD-OE2	5.04	1.31	1.25

All (302) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	330	ARG	NE-CZ-NH1	14.47	127.54	120.30
1	O	164	ARG	NE-CZ-NH1	13.08	126.84	120.30
1	C	15	TYR	CB-CG-CD2	12.78	128.66	121.00
1	C	15	TYR	CB-CG-CD1	-12.76	113.35	121.00
1	C	91	PHE	CB-CG-CD1	12.10	129.27	120.80
1	C	267	ASP	CB-CG-OD2	-12.04	107.46	118.30
1	O	139	ARG	CD-NE-CZ	12.03	140.45	123.60
1	C	165	ASP	CB-CG-OD2	-11.28	108.14	118.30
1	O	330	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	O	65	ASP	CB-CG-OD2	-11.16	108.26	118.30
1	O	20	TYR	CB-CG-CD1	11.05	127.63	121.00
1	O	161	TYR	CB-CG-CD2	11.00	127.60	121.00
1	O	340	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	O	82	ARG	CD-NE-CZ	10.78	138.69	123.60
1	C	53	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	C	106	GLN	N-CA-CB	-10.01	92.58	110.60
1	C	290	TYR	CB-CG-CD1	-9.94	115.04	121.00
1	O	254	ASP	CB-CG-OD2	-9.93	109.36	118.30
1	O	65	ASP	CB-CG-OD1	9.85	127.17	118.30
1	O	95	ASP	CB-CG-OD2	-9.79	109.48	118.30
1	C	164	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	O	82	ARG	NE-CZ-NH2	9.76	125.18	120.30
1	C	267	ASP	CB-CG-OD1	9.75	127.07	118.30
1	C	53	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	O	156	ASP	CB-CG-OD1	9.62	126.96	118.30
1	O	165	ASP	CB-CG-OD1	9.54	126.88	118.30
1	C	253	PHE	CB-CG-CD1	-9.50	114.15	120.80
1	O	307	PRO	N-CA-CB	9.36	114.53	103.30
1	O	165	ASP	N-CA-CB	9.32	127.39	110.60
1	C	75	ASN	N-CA-CB	9.22	127.20	110.60
1	O	95	ASP	CB-CG-OD1	9.10	126.49	118.30
1	O	156	ASP	CB-CG-OD2	-9.06	110.15	118.30
1	C	16	MET	CA-CB-CG	-8.97	98.04	113.30
1	O	119	PHE	N-CA-C	8.96	135.20	111.00
1	O	21	TYR	CB-CG-CD1	-8.94	115.64	121.00
1	O	218	GLU	N-CA-CB	8.89	126.59	110.60
1	C	251	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	O	251	ARG	N-CA-CB	8.79	126.42	110.60
1	C	219	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	O	172	LEU	C-N-CA	-8.77	103.88	122.30
1	O	216	LEU	N-CA-CB	-8.72	92.97	110.40
1	O	139	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	O	73	LYS	CB-CA-C	8.60	127.60	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	PHE	CB-CG-CD2	-8.59	114.79	120.80
1	O	338	LEU	CB-CA-C	-8.54	93.97	110.20
1	O	60	TYR	N-CA-CB	-8.31	95.65	110.60
1	O	34	LYS	CB-CA-C	-8.29	93.81	110.40
1	O	125	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	O	171	SER	CB-CA-C	-8.23	94.46	110.10
1	O	254	ASP	CB-CG-OD1	8.15	125.64	118.30
1	C	165	ASP	CB-CG-OD1	8.15	125.63	118.30
1	O	120	MET	CB-CA-C	8.13	126.66	110.40
1	C	161	TYR	CB-CG-CD2	8.11	125.87	121.00
1	O	231	TYR	CB-CG-CD2	7.95	125.77	121.00
1	O	145	ASP	CB-CG-OD1	7.93	125.43	118.30
1	C	68	ASP	CB-CG-OD1	7.87	125.38	118.30
1	O	15	TYR	CB-CG-CD1	7.84	125.71	121.00
1	C	290	TYR	N-CA-CB	7.84	124.71	110.60
1	O	60	TYR	CA-CB-CG	-7.81	98.57	113.40
1	O	55	TYR	CB-CG-CD2	-7.80	116.32	121.00
1	C	330	ARG	N-CA-CB	7.79	124.62	110.60
1	C	161	TYR	CB-CG-CD1	-7.78	116.33	121.00
1	O	20	TYR	CB-CG-CD2	-7.74	116.36	121.00
1	C	217	CYS	N-CA-CB	7.64	124.36	110.60
1	C	68	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	O	339	ALA	N-CA-CB	7.61	120.75	110.10
1	C	121	LEU	CB-CA-C	-7.57	95.81	110.20
1	O	121	LEU	CA-CB-CG	-7.57	97.90	115.30
1	O	163	ASN	N-CA-CB	7.55	124.20	110.60
1	O	72	TYR	CG-CD1-CE1	-7.53	115.28	121.30
1	O	233	SER	CB-CA-C	-7.53	95.80	110.10
1	O	164	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	C	79	LEU	N-CA-CB	-7.51	95.38	110.40
1	O	58	CYS	CA-CB-SG	-7.48	100.53	114.00
1	O	159	SER	N-CA-CB	-7.46	99.31	110.50
1	C	160	PHE	CB-CA-C	-7.45	95.50	110.40
1	O	333	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	C	219	ASP	CB-CG-OD1	7.37	124.93	118.30
1	C	84	SER	N-CA-CB	-7.37	99.45	110.50
1	C	68	ASP	N-CA-CB	-7.35	97.37	110.60
1	O	106	GLN	CB-CA-C	-7.31	95.77	110.40
1	O	83	TYR	CG-CD2-CE2	-7.30	115.46	121.30
1	O	304	ASP	CB-CG-OD1	7.30	124.87	118.30
1	C	125	ASP	CB-CG-OD1	7.26	124.84	118.30
1	O	332	ASN	CB-CA-C	-7.25	95.89	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	340	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	C	333	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	253	PHE	CB-CG-CD2	7.10	125.77	120.80
1	O	52	SER	CB-CA-C	-7.09	96.62	110.10
1	O	238	SER	CB-CA-C	7.08	123.56	110.10
1	C	309	THR	N-CA-CB	-7.08	96.84	110.30
1	C	268	ILE	CA-CB-CG1	-7.06	97.59	111.00
1	O	154	LYS	N-CA-CB	7.05	123.30	110.60
1	C	198	THR	CA-CB-CG2	-7.05	102.53	112.40
1	O	210	VAL	CA-C-N	-6.99	102.22	116.20
1	C	272	LEU	N-CA-CB	-6.96	96.48	110.40
1	O	187	GLU	CB-CG-CD	-6.96	95.42	114.20
1	C	294	LYS	CB-CA-C	-6.94	96.51	110.40
1	O	104	VAL	CB-CA-C	-6.94	98.22	111.40
1	C	320	ILE	CB-CA-C	-6.92	97.76	111.60
1	O	67	SER	CA-C-N	-6.91	102.00	117.20
1	C	11	ILE	CA-CB-CG1	-6.91	97.87	111.00
1	O	330	ARG	CD-NE-CZ	6.90	133.26	123.60
1	C	139	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	O	6	THR	N-CA-C	6.82	129.41	111.00
1	O	200	VAL	CB-CA-C	-6.82	98.45	111.40
1	O	333	ARG	CD-NE-CZ	-6.81	114.07	123.60
1	C	251	ARG	CG-CD-NE	6.79	126.07	111.80
1	C	158	PHE	CB-CG-CD1	-6.79	116.05	120.80
1	O	72	TYR	CA-CB-CG	-6.79	100.50	113.40
1	C	196	ILE	N-CA-CB	-6.77	95.22	110.80
1	C	65	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	C	153	LEU	C-N-CA	-6.75	104.81	121.70
1	O	165	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	C	250	LYS	N-CA-C	6.73	129.18	111.00
1	C	127	VAL	CA-CB-CG2	-6.71	100.83	110.90
1	O	340	ARG	CD-NE-CZ	-6.70	114.22	123.60
1	C	166	SER	N-CA-CB	6.69	120.54	110.50
1	O	328	ASP	N-CA-CB	-6.68	98.58	110.60
1	O	69	SER	N-CA-CB	6.67	120.51	110.50
1	O	272	LEU	CB-CG-CD1	-6.60	99.78	111.00
1	O	324	TYR	N-CA-CB	-6.59	98.73	110.60
1	C	238	SER	CB-CA-C	-6.58	97.59	110.10
1	O	253	PHE	CB-CG-CD1	6.58	125.40	120.80
1	C	327	PHE	CG-CD1-CE1	-6.55	113.59	120.80
1	O	83	TYR	CD1-CE1-CZ	-6.54	113.91	119.80
1	O	283	ASP	CB-CG-OD2	-6.52	112.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	337	ALA	CB-CA-C	-6.50	100.35	110.10
1	C	124	PHE	CB-CG-CD2	6.50	125.35	120.80
1	O	172	LEU	N-CA-CB	-6.49	97.42	110.40
1	O	141	THR	CA-CB-CG2	-6.49	103.32	112.40
1	O	253	PHE	N-CA-CB	-6.49	98.92	110.60
1	O	328	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	O	74	HIS	CB-CA-C	-6.44	97.52	110.40
1	O	162	TYR	CB-CG-CD1	6.39	124.84	121.00
1	O	243	MET	N-CA-CB	-6.38	99.11	110.60
1	C	94	GLN	N-CA-CB	6.36	122.04	110.60
1	O	68	ASP	N-CA-C	-6.35	93.86	111.00
1	C	73	LYS	N-CA-CB	-6.34	99.18	110.60
1	C	307	PRO	CA-N-CD	-6.33	102.63	111.50
1	C	38	ASP	CB-CA-C	-6.33	97.73	110.40
1	O	118	PRO	C-N-CA	6.31	137.47	121.70
1	O	340	ARG	N-CA-CB	-6.30	99.27	110.60
1	O	97	ILE	CA-CB-CG1	-6.23	99.16	111.00
1	C	259	CYS	N-CA-C	6.23	127.83	111.00
1	O	333	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	C	264	THR	N-CA-CB	-6.23	98.47	110.30
1	O	88	VAL	N-CA-C	-6.21	94.22	111.00
1	O	305	ILE	CB-CA-C	6.21	124.03	111.60
1	O	306	PRO	O-C-N	6.21	132.91	121.10
1	O	329	ARG	CD-NE-CZ	6.20	132.27	123.60
1	O	112	THR	N-CA-CB	6.19	122.05	110.30
1	C	26	ILE	CB-CA-C	-6.18	99.24	111.60
1	C	164	ARG	C-N-CA	-6.16	106.29	121.70
1	C	62	LYS	CB-CA-C	-6.16	98.08	110.40
1	C	202	GLN	N-CA-CB	-6.16	99.51	110.60
1	C	324	TYR	CG-CD1-CE1	6.15	126.22	121.30
1	C	164	ARG	CD-NE-CZ	6.14	132.20	123.60
1	C	197	LYS	CB-CG-CD	6.09	127.43	111.60
1	O	284	TYR	CG-CD2-CE2	-6.08	116.44	121.30
1	O	322	LYS	N-CA-CB	6.07	121.53	110.60
1	C	28	THR	C-N-CD	-6.05	107.28	120.60
1	O	202	GLN	CA-CB-CG	6.04	126.69	113.40
1	O	145	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	O	283	ASP	CB-CG-OD1	6.02	123.72	118.30
1	O	304	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	O	143	ILE	C-N-CA	-5.99	106.72	121.70
1	C	251	ARG	CD-NE-CZ	5.96	131.95	123.60
1	C	50	LYS	CA-CB-CG	5.95	126.49	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	186	TYR	C-N-CA	-5.94	106.85	121.70
1	C	156	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	O	232	ILE	N-CA-C	-5.92	95.01	111.00
1	C	75	ASN	C-N-CA	-5.92	109.88	122.30
1	O	125	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	288	GLU	CB-CG-CD	5.90	130.14	114.20
1	C	327	PHE	CG-CD2-CE2	5.89	127.28	120.80
1	C	329	ARG	CG-CD-NE	-5.87	99.47	111.80
1	O	307	PRO	N-CA-C	5.87	127.35	112.10
1	O	141	THR	CB-CA-C	-5.86	95.77	111.60
1	C	9	SER	C-N-CA	-5.86	107.06	121.70
1	C	19	GLN	CB-CG-CD	-5.85	96.40	111.60
1	C	267	ASP	CB-CA-C	-5.84	98.72	110.40
1	O	256	VAL	CA-C-N	-5.83	104.37	117.20
1	O	250	LYS	C-N-CA	-5.82	107.15	121.70
1	O	201	TRP	N-CA-CB	5.81	121.06	110.60
1	C	226	ASP	N-CA-CB	-5.79	100.18	110.60
1	O	187	GLU	CG-CD-OE2	-5.79	106.72	118.30
1	O	219	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	172	LEU	CA-CB-CG	-5.77	102.03	115.30
1	O	284	TYR	CD1-CE1-CZ	-5.75	114.62	119.80
1	C	327	PHE	CB-CG-CD2	-5.75	116.77	120.80
1	C	206	LYS	N-CA-C	5.75	126.52	111.00
1	C	333	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	O	323	PHE	CD1-CG-CD2	5.74	125.76	118.30
1	O	19	GLN	N-CA-CB	-5.72	100.30	110.60
1	C	252	LEU	N-CA-CB	5.71	121.83	110.40
1	C	88	VAL	N-CA-C	-5.71	95.58	111.00
1	O	118	PRO	CB-CA-C	-5.71	97.72	112.00
1	O	176	ILE	CB-CA-C	-5.70	100.20	111.60
1	O	162	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	C	301	HIS	CB-CA-C	-5.69	99.01	110.40
1	O	336	PHE	CB-CG-CD1	5.69	124.79	120.80
1	O	165	ASP	O-C-N	5.68	131.79	122.70
1	C	79	LEU	CB-CG-CD1	-5.68	101.35	111.00
1	O	219	ASP	CB-CA-C	5.67	121.75	110.40
1	C	95	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	C	56	THR	CB-CA-C	5.66	126.89	111.60
1	C	43	ASN	N-CA-CB	-5.65	100.43	110.60
1	C	283	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	10	VAL	CA-CB-CG2	-5.63	102.45	110.90
1	C	327	PHE	CZ-CE2-CD2	-5.58	113.41	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	LEU	N-CA-C	-5.58	95.94	111.00
1	O	329	ARG	CG-CD-NE	5.57	123.49	111.80
1	O	158	PHE	N-CA-CB	5.56	120.61	110.60
1	C	115	PRO	N-CA-CB	5.56	109.97	103.30
1	O	119	PHE	N-CA-CB	5.56	120.61	110.60
1	C	125	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	269	SER	CB-CA-C	5.54	120.63	110.10
1	C	47	PRO	N-CA-CB	5.54	109.95	103.30
1	O	253	PHE	CA-C-N	5.54	129.38	117.20
1	O	291	SER	CB-CA-C	-5.53	99.59	110.10
1	O	323	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	C	308	PRO	N-CA-C	-5.51	97.77	112.10
1	C	231	TYR	CG-CD2-CE2	5.51	125.71	121.30
1	O	31	GLN	CB-CA-C	-5.50	99.40	110.40
1	O	83	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	O	157	VAL	N-CA-CB	-5.50	99.40	111.50
1	C	293	LYS	CB-CG-CD	5.48	125.86	111.60
1	O	271	HIS	C-N-CA	-5.48	108.01	121.70
1	C	226	ASP	CA-CB-CG	5.47	125.44	113.40
1	C	233	SER	CB-CA-C	-5.47	99.70	110.10
1	C	117	LEU	N-CA-CB	-5.47	99.46	110.40
1	C	41	SER	C-N-CA	-5.46	108.05	121.70
1	O	185	HIS	N-CA-C	5.45	125.71	111.00
1	C	203	ILE	CG1-CB-CG2	5.45	123.38	111.40
1	O	327	PHE	CZ-CE2-CD2	-5.44	113.57	120.10
1	C	327	PHE	CD1-CE1-CZ	5.44	126.63	120.10
1	O	202	GLN	N-CA-CB	-5.42	100.83	110.60
1	O	253	PHE	N-CA-C	-5.42	96.37	111.00
1	O	292	SER	N-CA-CB	-5.42	102.37	110.50
1	O	84	SER	CB-CA-C	-5.42	99.81	110.10
1	O	276	GLU	CA-CB-CG	5.41	125.30	113.40
1	C	281	SER	N-CA-CB	-5.41	102.39	110.50
1	C	290	TYR	CZ-CE2-CD2	-5.41	114.93	119.80
1	O	122	ALA	N-CA-CB	-5.41	102.53	110.10
1	C	325	THR	CA-CB-CG2	5.39	119.95	112.40
1	O	176	ILE	CA-CB-CG1	-5.38	100.78	111.00
1	O	310	GLY	N-CA-C	-5.38	99.66	113.10
1	C	119	PHE	N-CA-C	5.37	125.49	111.00
1	O	66	ALA	N-CA-CB	5.36	117.60	110.10
1	O	146	ASN	N-CA-CB	5.36	120.24	110.60
1	C	123	GLU	CG-CD-OE2	-5.35	107.61	118.30
1	C	87	THR	N-CA-CB	-5.34	100.16	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	121	LEU	CB-CA-C	-5.33	100.06	110.20
1	C	11	ILE	CB-CA-C	5.33	122.25	111.60
1	C	218	GLU	N-CA-C	5.32	125.38	111.00
1	O	164	ARG	CD-NE-CZ	5.32	131.04	123.60
1	C	68	ASP	CA-CB-CG	5.31	125.09	113.40
1	O	79	LEU	N-CA-CB	-5.28	99.85	110.40
1	O	268	ILE	N-CA-C	-5.28	96.76	111.00
1	C	93	SER	CB-CA-C	5.27	120.11	110.10
1	C	38	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	163	ASN	N-CA-CB	-5.24	101.17	110.60
1	O	256	VAL	O-C-N	5.23	131.07	122.70
1	C	123	GLU	CB-CG-CD	-5.23	100.09	114.20
1	O	161	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	O	195	LEU	CB-CG-CD2	5.21	119.86	111.00
1	O	194	ASN	N-CA-C	5.21	125.06	111.00
1	C	291	SER	N-CA-C	5.21	125.06	111.00
1	C	48	SER	O-C-N	5.20	131.01	122.70
1	O	241	LYS	CD-CE-NZ	5.20	123.65	111.70
1	O	219	ASP	C-N-CA	5.19	133.19	122.30
1	C	144	PHE	CB-CG-CD2	5.18	124.43	120.80
1	O	88	VAL	CB-CA-C	5.18	121.24	111.40
1	O	23	GLU	CG-CD-OE2	-5.18	107.95	118.30
1	C	75	ASN	CB-CA-C	5.17	120.75	110.40
1	C	329	ARG	CB-CA-C	-5.16	100.08	110.40
1	C	114	MET	CG-SD-CE	5.16	108.45	100.20
1	C	290	TYR	CG-CD1-CE1	-5.15	117.18	121.30
1	C	5	ASN	N-CA-CB	5.15	119.87	110.60
1	C	85	THR	N-CA-C	5.14	124.88	111.00
1	O	23	GLU	CB-CG-CD	-5.12	100.38	114.20
1	C	201	TRP	CB-CG-CD2	5.11	133.24	126.60
1	O	205	MET	CA-C-N	-5.11	105.97	117.20
1	O	238	SER	N-CA-CB	5.09	118.14	110.50
1	O	28	THR	CA-CB-CG2	-5.08	105.29	112.40
1	O	46	VAL	CB-CA-C	-5.07	101.77	111.40
1	O	307	PRO	CA-N-CD	-5.07	104.41	111.50
1	O	201	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	C	176	ILE	CB-CA-C	-5.05	101.50	111.60
1	O	67	SER	C-N-CA	5.05	134.33	121.70
1	C	61	HIS	N-CA-CB	-5.05	101.52	110.60
1	O	164	ARG	CA-C-N	5.03	128.27	117.20
1	C	204	GLN	N-CA-CB	-5.03	101.55	110.60
1	O	279	LEU	CB-CG-CD1	-5.02	102.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	161	TYR	CG-CD2-CE2	5.01	125.31	121.30
1	O	45	TRP	O-C-N	5.01	130.72	122.70
1	O	162	TYR	CA-CB-CG	5.01	122.92	113.40
1	O	72	TYR	CD1-CE1-CZ	5.01	124.31	119.80
1	C	211	GLY	N-CA-C	-5.00	100.59	113.10
1	O	69	SER	CA-C-N	-5.00	106.19	117.20
1	O	124	PHE	CB-CG-CD1	5.00	124.30	120.80

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	56	THR	CA
1	C	75	ASN	CA
1	C	203	ILE	CB
1	C	206	LYS	CA
1	C	259	CYS	CA
1	O	119	PHE	CA
1	O	194	ASN	CA
1	O	307	PRO	CA

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	C	2567	0	2498	241	0
1	O	2557	0	2489	282	0
2	C	34	0	48	22	0
2	O	34	0	48	9	0
All	All	5192	0	5083	524	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 51.

All (524) 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:260:ASN:HD22	1:C:261:GLU:N	1.41	1.16
1:C:216:LEU:HD12	1:C:238:SER:HB3	1.28	1.11
1:O:196:ILE:HG22	1:O:197:LYS:HG2	1.14	1.09
1:C:127:VAL:HG21	2:C:1341:C61:C19	1.83	1.09
1:C:96:ILE:HG22	1:C:105:THR:HG22	1.41	1.03
1:C:53:ARG:H	1:C:53:ARG:HD2	1.23	1.01
1:C:79:LEU:HD22	1:C:92:LEU:HD21	1.43	1.00
1:C:53:ARG:HD2	1:C:53:ARG:N	1.74	0.98
1:C:133:ILE:HG12	1:C:139:ARG:HH21	1.28	0.97
1:C:127:VAL:HG21	2:C:1341:C61:H191	1.46	0.95
1:C:133:ILE:HG12	1:C:139:ARG:NH2	1.82	0.94
1:C:127:VAL:CG2	2:C:1341:C61:H191	1.99	0.92
1:O:6:THR:H	1:O:154:LYS:HE3	1.35	0.92
1:O:59:VAL:HG12	1:O:60:TYR:CD2	2.07	0.89
1:O:216:LEU:HB2	1:O:241:LYS:NZ	1.88	0.88
1:O:106:GLN:NE2	1:O:146:ASN:HD22	1.70	0.88
1:C:96:ILE:HG22	1:C:105:THR:CG2	2.03	0.88
1:C:260:ASN:ND2	1:C:261:GLU:N	2.19	0.88
1:C:127:VAL:CG2	2:C:1341:C61:C19	2.52	0.87
1:C:47:PRO:HB3	1:C:114:MET:HE2	1.55	0.86
1:O:118:PRO:HG2	1:O:119:PHE:CD2	2.09	0.86
1:O:5:ASN:HA	1:O:154:LYS:CD	2.04	0.86
1:O:5:ASN:HA	1:O:154:LYS:HD2	1.57	0.86
1:O:279:LEU:HD22	1:O:283:ASP:HB3	1.56	0.85
1:C:84:SER:HB2	2:C:1341:C61:H261	1.58	0.84
1:C:156:ASP:H	1:C:330:ARG:HD2	1.40	0.84
1:O:216:LEU:HG	1:O:241:LYS:HE2	1.58	0.84
1:C:183:PRO:HA	1:C:186:TYR:CE1	2.13	0.83
1:C:196:ILE:HG23	1:C:197:LYS:N	1.92	0.83
1:O:209:SER:HB2	1:O:214:THR:HA	1.62	0.82
1:O:35:VAL:HG21	1:O:128:VAL:HG23	1.59	0.82
1:O:196:ILE:CG2	1:O:197:LYS:HG2	2.06	0.82
1:C:256:VAL:HG23	1:C:297:THR:HG22	1.61	0.82
1:O:82:ARG:O	2:O:1341:C61:H352	1.80	0.81
1:O:6:THR:N	1:O:154:LYS:HE3	1.94	0.81
1:O:216:LEU:CG	1:O:241:LYS:HE2	2.10	0.81
1:C:127:VAL:HG21	2:C:1341:C61:H192	1.59	0.81
1:O:196:ILE:HG22	1:O:197:LYS:CG	2.07	0.81
1:C:150:GLN:HB2	1:C:152:VAL:CG1	2.10	0.81
1:C:196:ILE:HG23	1:C:197:LYS:H	1.46	0.80
1:C:51:CYS:HB2	1:C:112:THR:HA	1.64	0.80
1:C:236:THR:O	1:C:240:GLU:HB2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:VAL:HG21	1:O:128:VAL:CG2	2.11	0.80
1:C:154:LYS:NZ	1:C:154:LYS:HB3	1.97	0.79
1:O:133:ILE:HD13	1:O:139:ARG:HD3	1.65	0.79
1:O:205:MET:CE	1:O:208:VAL:HG22	2.13	0.79
1:O:233:SER:HA	1:O:301:HIS:O	1.83	0.78
1:C:53:ARG:H	1:C:53:ARG:CD	1.97	0.78
1:O:195:LEU:HB2	1:O:332:ASN:O	1.82	0.78
1:O:216:LEU:HD23	1:O:217:CYS:H	1.48	0.78
1:O:251:ARG:HH11	1:O:253:PHE:H	1.31	0.78
1:O:285:VAL:HG22	1:O:298:LEU:HD22	1.65	0.78
1:O:57:ALA:HB3	1:O:114:MET:HB3	1.65	0.77
1:C:340:ARG:NH1	1:O:7:THR:HG22	2.00	0.77
1:O:291:SER:HB3	1:O:294:LYS:HG2	1.65	0.77
1:O:251:ARG:HH12	1:O:253:PHE:HB2	1.50	0.77
1:C:157:VAL:HG12	1:C:328:ASP:HA	1.67	0.76
1:O:205:MET:HE2	1:O:208:VAL:HG22	1.66	0.76
1:C:194:ASN:HA	1:C:333:ARG:HB3	1.66	0.76
1:O:79:LEU:HD13	1:O:92:LEU:HD13	1.67	0.76
1:O:133:ILE:CD1	1:O:139:ARG:HG3	2.16	0.75
1:O:58:CYS:SG	1:O:114:MET:HE3	2.26	0.75
1:C:261:GLU:O	1:C:264:THR:HB	1.86	0.75
1:C:239:ILE:HG13	1:C:301:HIS:O	1.86	0.75
1:O:72:TYR:HE1	1:O:93:SER:HG	1.33	0.75
1:C:206:LYS:HE2	1:C:271:HIS:NE2	2.01	0.75
1:C:16:MET:O	1:C:18:THR:HG23	1.86	0.74
1:O:153:LEU:O	1:O:154:LYS:HE2	1.87	0.74
1:O:47:PRO:HB2	1:O:63:LEU:HD23	1.70	0.74
1:O:139:ARG:NH2	1:O:139:ARG:HB2	2.03	0.74
1:C:26:ILE:HD13	1:C:97:ILE:HG12	1.70	0.74
1:O:306:PRO:O	1:O:308:PRO:HD2	1.88	0.74
1:O:214:THR:HG23	1:O:218:GLU:HG3	1.70	0.73
1:C:340:ARG:HH12	1:O:7:THR:HG22	1.51	0.73
1:O:283:ASP:OD1	1:O:322:LYS:HE2	1.88	0.73
1:C:150:GLN:HB2	1:C:152:VAL:HG11	1.72	0.72
1:C:260:ASN:HD22	1:C:261:GLU:H	1.36	0.72
1:C:106:GLN:OE1	1:C:146:ASN:ND2	2.23	0.71
1:O:205:MET:HE1	1:O:270:PHE:HD2	1.56	0.71
1:O:106:GLN:NE2	1:O:146:ASN:ND2	2.37	0.70
1:O:57:ALA:CB	1:O:114:MET:HB3	2.20	0.70
1:O:194:ASN:HB3	1:O:333:ARG:HB3	1.74	0.70
1:O:251:ARG:NH1	1:O:253:PHE:H	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:VAL:HG23	1:O:36:VAL:N	2.06	0.70
1:C:73:LYS:HB3	1:C:94:GLN:HG3	1.74	0.69
1:O:205:MET:CE	1:O:270:PHE:HD2	2.04	0.69
1:O:205:MET:O	1:O:220:GLY:HA2	1.92	0.69
1:C:260:ASN:ND2	1:C:261:GLU:H	1.87	0.69
1:C:216:LEU:HD12	1:C:238:SER:CB	2.15	0.69
1:O:84:SER:O	1:O:85:THR:HG23	1.93	0.69
1:O:53:ARG:HB2	1:O:59:VAL:HG22	1.74	0.69
1:O:55:TYR:OH	1:O:113:GLU:HG3	1.92	0.68
1:O:216:LEU:HB2	1:O:241:LYS:HZ3	1.58	0.68
1:C:156:ASP:H	1:C:330:ARG:CD	2.05	0.68
1:O:115:PRO:HB2	1:O:118:PRO:CD	2.22	0.68
1:O:33:PHE:CE2	1:O:62:LYS:HG2	2.29	0.68
1:C:47:PRO:CB	1:C:114:MET:HE2	2.24	0.68
1:C:150:GLN:HB2	1:C:152:VAL:HG12	1.76	0.68
1:C:200:VAL:CG1	1:C:202:GLN:HB2	2.23	0.68
1:O:251:ARG:NH1	1:O:253:PHE:O	2.26	0.68
1:C:232:ILE:O	1:C:300:ILE:HA	1.93	0.67
2:O:1341:C61:H162	2:O:1341:C61:N23	2.10	0.67
1:C:215:LEU:HB3	1:C:216:LEU:HD22	1.77	0.67
1:O:139:ARG:HB2	1:O:139:ARG:HH21	1.59	0.67
1:C:154:LYS:HZ2	1:C:154:LYS:HB3	1.58	0.66
1:O:205:MET:HE2	1:O:208:VAL:CG2	2.26	0.66
1:C:14:ASN:ND2	1:C:165:ASP:HB2	2.09	0.66
1:O:106:GLN:HE21	1:O:146:ASN:ND2	1.91	0.66
1:O:305:ILE:O	1:O:310:GLY:HA3	1.95	0.66
1:C:47:PRO:HG3	1:C:114:MET:HE1	1.77	0.66
1:C:57:ALA:HA	1:C:120:MET:CE	2.26	0.65
1:C:153:LEU:HD22	1:C:179:GLY:HA3	1.79	0.65
1:C:305:ILE:O	1:C:310:GLY:HA3	1.96	0.65
1:C:79:LEU:HD22	1:C:92:LEU:CD2	2.24	0.65
1:O:6:THR:O	1:O:154:LYS:N	2.30	0.65
1:C:47:PRO:HG3	1:C:114:MET:CE	2.26	0.65
1:C:17:ASP:OD1	1:C:165:ASP:HB3	1.97	0.65
1:O:193:ILE:HD12	1:O:273:GLY:HA3	1.79	0.64
1:O:5:ASN:CA	1:O:154:LYS:HE3	2.28	0.64
1:C:242:LEU:HD11	1:C:246:LEU:HD11	1.78	0.64
1:O:133:ILE:HD11	1:O:139:ARG:HG3	1.79	0.64
1:C:307:PRO:HA	1:C:310:GLY:O	1.97	0.64
1:O:284:TYR:CD1	1:O:285:VAL:HG23	2.33	0.64
1:C:164:ARG:HH21	1:O:172:LEU:HD13	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:133:ILE:HD13	1:O:139:ARG:HG3	1.78	0.63
1:O:92:LEU:HD21	1:O:140:VAL:HG21	1.80	0.63
1:O:9:SER:HA	1:O:176:ILE:O	1.99	0.63
1:O:260:ASN:HB2	1:O:292:SER:HA	1.80	0.63
1:O:289:SER:OG	1:O:294:LYS:HD3	2.00	0.62
1:O:164:ARG:O	1:O:166:SER:N	2.32	0.62
1:O:117:LEU:HD12	1:O:117:LEU:O	1.99	0.62
1:C:216:LEU:N	1:C:216:LEU:HD23	2.15	0.61
1:O:34:LYS:CB	1:O:124:PHE:HA	2.30	0.61
1:O:66:ALA:HB1	1:O:72:TYR:CG	2.36	0.61
1:C:198:THR:HB	1:C:332:ASN:ND2	2.15	0.60
1:O:115:PRO:HB2	1:O:118:PRO:HD2	1.81	0.60
1:C:118:PRO:HB2	2:C:1341:C61:H9C3	1.82	0.60
1:C:139:ARG:HG3	1:C:139:ARG:O	2.01	0.60
1:O:118:PRO:CD	1:O:119:PHE:H	2.12	0.60
1:O:79:LEU:CD1	1:O:92:LEU:HD13	2.31	0.60
1:C:193:ILE:HD13	1:C:203:ILE:CD1	2.31	0.60
1:O:115:PRO:HB2	1:O:118:PRO:HD3	1.83	0.60
1:C:192:TYR:HA	1:C:335:GLY:HA2	1.84	0.60
1:O:45:TRP:CE3	1:O:111:VAL:HG21	2.37	0.59
1:O:34:LYS:HB2	1:O:124:PHE:HA	1.83	0.59
1:O:83:TYR:HD1	2:O:1341:C61:H321	1.66	0.59
1:O:5:ASN:C	1:O:154:LYS:HG2	2.22	0.59
1:O:38:ASP:OD1	1:O:228:GLY:HA3	2.02	0.59
1:C:249:LYS:O	1:C:255:TYR:HA	2.02	0.59
1:O:52:SER:OG	1:O:54:LEU:HB2	2.03	0.59
1:C:306:PRO:O	1:C:308:PRO:N	2.36	0.59
1:C:308:PRO:HB2	1:C:309:THR:HG23	1.85	0.59
1:O:216:LEU:HD12	1:O:241:LYS:CE	2.33	0.59
1:O:92:LEU:HD12	1:O:108:PHE:O	2.03	0.59
1:C:195:LEU:HB2	1:C:332:ASN:O	2.03	0.58
1:O:55:TYR:CE1	1:O:113:GLU:HA	2.37	0.58
1:O:210:VAL:HG21	1:O:242:LEU:HD12	1.85	0.58
1:O:139:ARG:CB	1:O:139:ARG:HH21	2.16	0.58
1:O:34:LYS:HB2	1:O:124:PHE:CA	2.34	0.58
1:O:5:ASN:HA	1:O:154:LYS:CE	2.34	0.58
1:O:197:LYS:O	1:O:197:LYS:HG3	2.03	0.58
1:O:227:THR:O	2:O:1341:C61:H2C2	2.03	0.58
1:C:157:VAL:CG1	1:C:328:ASP:HA	2.34	0.58
1:O:72:TYR:HE1	1:O:93:SER:OG	1.86	0.58
1:C:260:ASN:HD22	1:C:260:ASN:C	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:PHE:HE1	1:C:336:PHE:CE2	2.22	0.57
1:O:251:ARG:HD2	1:O:252:LEU:H	1.68	0.57
1:O:115:PRO:C	1:O:117:LEU:H	2.08	0.57
1:O:234:GLY:O	1:O:303:MET:N	2.33	0.57
1:C:20:TYR:HB2	2:C:1341:C61:H2C1	1.85	0.57
1:O:26:ILE:HG12	1:O:97:ILE:HG12	1.86	0.57
1:O:52:SER:OG	1:O:54:LEU:N	2.31	0.57
1:C:57:ALA:HA	1:C:120:MET:HE3	1.87	0.57
1:O:272:LEU:HD23	1:O:277:TYR:CD1	2.39	0.57
1:O:6:THR:HG23	1:O:7:THR:N	2.20	0.57
1:C:53:ARG:HB2	1:C:59:VAL:CG1	2.35	0.57
1:C:5:ASN:C	1:C:5:ASN:HD22	2.06	0.57
1:O:133:ILE:HD13	1:O:139:ARG:CD	2.34	0.57
1:O:106:GLN:HE21	1:O:146:ASN:HD22	1.42	0.57
1:O:251:ARG:CG	1:O:252:LEU:H	2.15	0.56
1:C:99:VAL:O	1:C:99:VAL:HG23	2.05	0.56
1:O:133:ILE:HG13	1:O:142:PRO:HD3	1.85	0.56
1:O:216:LEU:CD2	1:O:217:CYS:H	2.19	0.56
1:O:279:LEU:CD2	1:O:283:ASP:HB3	2.30	0.56
2:O:1341:C61:H18	2:O:1341:C61:C10	2.36	0.56
1:C:130:MET:HA	1:C:130:MET:HE3	1.87	0.56
1:C:96:ILE:HA	1:C:105:THR:HA	1.86	0.56
1:O:48:SER:O	1:O:63:LEU:HD22	2.06	0.56
1:O:25:GLY:O	1:O:97:ILE:HA	2.06	0.56
1:O:91:PHE:HE1	1:O:112:THR:CG2	2.19	0.56
1:C:226:ASP:OD1	1:C:229:ALA:HB2	2.07	0.55
1:C:57:ALA:CB	1:C:114:MET:HG2	2.36	0.55
1:C:256:VAL:HG13	1:C:295:LEU:HD22	1.87	0.55
1:C:206:LYS:NZ	1:C:273:GLY:N	2.54	0.55
1:O:47:PRO:HD3	1:O:125:ASP:O	2.06	0.55
1:O:64:PHE:CE1	1:O:108:PHE:HZ	2.24	0.55
1:C:206:LYS:HE2	1:C:271:HIS:CD2	2.41	0.55
1:O:34:LYS:HG3	1:O:124:PHE:HA	1.89	0.55
1:O:155:GLU:HG3	1:O:179:GLY:O	2.05	0.55
1:O:272:LEU:CD2	1:O:277:TYR:CD1	2.89	0.55
1:O:340:ARG:HH21	1:O:340:ARG:HB3	1.71	0.55
1:C:83:TYR:CE2	2:C:1341:C61:C20	2.90	0.55
1:O:206:LYS:NZ	1:O:274:GLY:HA2	2.21	0.55
1:C:18:THR:O	1:C:230:SER:HB3	2.06	0.55
1:C:216:LEU:C	1:C:218:GLU:H	2.10	0.55
1:C:118:PRO:HG2	2:C:1341:C61:H13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:250:LYS:HA	1:O:255:TYR:HA	1.88	0.55
1:C:96:ILE:CG2	1:C:105:THR:HG22	2.27	0.54
1:C:242:LEU:CD1	1:C:246:LEU:HD11	2.37	0.54
1:O:45:TRP:NE1	1:O:127:VAL:CG1	2.71	0.54
1:C:73:LYS:CB	1:C:94:GLN:HG3	2.36	0.54
1:O:92:LEU:HG	1:O:107:MET:HG3	1.89	0.54
1:O:104:VAL:HG12	1:O:105:THR:N	2.21	0.54
1:O:15:TYR:CD1	1:O:16:MET:HG3	2.43	0.54
1:O:251:ARG:CD	1:O:252:LEU:H	2.21	0.54
1:O:24:ILE:HG12	1:O:35:VAL:HG11	1.89	0.54
1:C:256:VAL:HG23	1:C:297:THR:CG2	2.35	0.54
1:O:227:THR:HG22	1:O:320:ILE:HD13	1.90	0.54
1:C:253:PHE:O	1:C:301:HIS:CE1	2.61	0.54
1:O:210:VAL:CG2	1:O:242:LEU:HD12	2.38	0.54
1:O:38:ASP:O	1:O:130:MET:N	2.28	0.54
1:C:118:PRO:HB2	2:C:1341:C61:H13	1.89	0.54
1:C:294:LYS:NZ	1:C:294:LYS:HB3	2.23	0.54
1:C:8:SER:O	1:C:177:VAL:HA	2.08	0.54
1:C:151:GLY:C	1:C:152:VAL:HG12	2.28	0.53
1:O:16:MET:O	1:O:17:ASP:HB2	2.08	0.53
1:O:47:PRO:CB	1:O:63:LEU:HD23	2.37	0.53
1:C:196:ILE:HG21	1:C:202:GLN:HB3	1.89	0.53
1:C:258:LYS:HB3	1:C:261:GLU:CD	2.28	0.53
1:C:306:PRO:HB2	1:C:308:PRO:HD2	1.90	0.53
1:C:132:PHE:CD2	1:C:200:VAL:N	2.77	0.53
1:C:213:SER:O	1:C:215:LEU:N	2.42	0.53
1:C:200:VAL:HG11	1:C:202:GLN:HB2	1.89	0.53
1:C:211:GLY:HA2	1:C:266:PRO:HB2	1.91	0.53
1:C:320:ILE:O	1:C:320:ILE:HG22	2.09	0.53
1:C:59:VAL:HG23	1:C:60:TYR:CD1	2.43	0.53
1:C:8:SER:O	1:C:178:LEU:N	2.33	0.53
1:O:232:ILE:HG13	1:O:318:THR:HB	1.91	0.53
1:O:202:GLN:OE1	1:O:222:LEU:HD13	2.09	0.53
1:O:58:CYS:O	1:O:63:LEU:HD11	2.09	0.53
1:O:205:MET:HE1	1:O:270:PHE:CD2	2.42	0.53
1:C:72:TYR:CG	1:C:73:LYS:N	2.77	0.53
1:O:83:TYR:HB3	2:O:1341:C61:H22	1.91	0.52
1:C:256:VAL:CG2	1:C:297:THR:HG22	2.35	0.52
1:C:158:PHE:CE2	1:C:327:PHE:CD1	2.98	0.52
1:C:62:LYS:NZ	1:C:62:LYS:HB3	2.22	0.52
1:O:161:TYR:HE2	1:O:172:LEU:CD2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:5:ASN:N	1:O:154:LYS:HE3	2.24	0.52
1:C:53:ARG:HB2	1:C:59:VAL:HG12	1.89	0.52
1:O:340:ARG:O	1:O:340:ARG:HD2	2.10	0.52
1:C:265:LEU:HB3	1:C:284:TYR:OH	2.09	0.52
1:C:306:PRO:HG2	1:C:308:PRO:HG2	1.91	0.52
1:O:41:SER:O	1:O:131:GLY:N	2.42	0.52
1:O:45:TRP:CE2	1:O:127:VAL:HG12	2.44	0.52
1:O:206:LYS:HZ3	1:O:274:GLY:HA2	1.75	0.52
1:O:291:SER:HB3	1:O:294:LYS:CG	2.37	0.52
1:O:65:ASP:O	1:O:68:ASP:HB2	2.10	0.52
1:C:196:ILE:CG2	1:C:197:LYS:N	2.68	0.52
1:C:202:GLN:OE1	1:C:312:THR:OG1	2.27	0.52
1:O:137:ILE:HG22	1:O:137:ILE:O	2.08	0.52
1:O:253:PHE:O	1:O:254:ASP:O	2.28	0.52
1:O:59:VAL:HG12	1:O:60:TYR:CE2	2.44	0.52
1:C:64:PHE:CE1	1:C:66:ALA:HB2	2.45	0.51
1:C:192:TYR:HB3	1:C:333:ARG:HD2	1.93	0.51
1:C:286:PHE:CE1	1:C:299:ALA:HB2	2.45	0.51
1:C:206:LYS:HZ1	1:C:273:GLY:N	2.09	0.51
1:O:139:ARG:HA	1:O:139:ARG:HH21	1.76	0.51
1:C:206:LYS:HZ1	1:C:273:GLY:CA	2.24	0.51
1:O:236:THR:OG1	1:O:304:ASP:OD2	2.29	0.51
1:O:34:LYS:CG	1:O:124:PHE:HA	2.40	0.51
1:O:26:ILE:CD1	1:O:46:VAL:HG11	2.39	0.51
1:O:310:GLY:HA2	1:O:312:THR:HG22	1.92	0.51
1:O:300:ILE:O	1:O:301:HIS:HD2	1.92	0.51
1:O:217:CYS:O	1:O:217:CYS:SG	2.68	0.51
1:C:120:MET:HE3	1:C:120:MET:HA	1.93	0.51
1:C:192:TYR:CD2	1:C:335:GLY:HA3	2.46	0.51
1:C:284:TYR:CD1	1:C:285:VAL:HG23	2.45	0.51
1:C:19:GLN:HG2	2:C:1341:C61:H5C1	1.94	0.50
1:C:250:LYS:O	1:C:252:LEU:N	2.44	0.50
1:O:88:VAL:HG12	1:O:115:PRO:HD2	1.92	0.50
1:C:45:TRP:HA	1:C:109:GLY:O	2.11	0.50
1:C:127:VAL:HG23	2:C:1341:C61:H191	1.86	0.50
1:C:248:ALA:HB1	1:C:256:VAL:H	1.77	0.50
1:C:94:GLN:HB3	1:C:107:MET:CE	2.42	0.50
1:O:35:VAL:CG2	1:O:128:VAL:HG23	2.36	0.50
1:O:305:ILE:O	1:O:311:PRO:HA	2.11	0.50
1:O:97:ILE:HD12	1:O:106:GLN:HB2	1.92	0.50
1:O:216:LEU:HD12	1:O:241:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ARG:HB3	1:C:254:ASP:OD2	2.12	0.50
1:O:154:LYS:HA	1:O:154:LYS:HE2	1.93	0.50
1:O:246:LEU:HD12	1:O:298:LEU:HD11	1.93	0.50
1:O:234:GLY:O	1:O:302:ALA:HA	2.11	0.50
1:C:19:GLN:HE22	1:C:123:GLU:HB2	1.76	0.50
1:C:6:THR:HG22	1:C:7:THR:N	2.27	0.50
1:O:287:GLN:C	1:O:289:SER:H	2.15	0.49
1:O:59:VAL:HG12	1:O:60:TYR:CG	2.47	0.49
1:O:300:ILE:C	1:O:301:HIS:HD2	2.15	0.49
1:C:97:ILE:HG22	1:C:98:THR:N	2.27	0.49
1:O:133:ILE:HD13	1:O:139:ARG:CG	2.42	0.49
1:C:92:LEU:O	1:C:93:SER:HB3	2.13	0.49
1:C:133:ILE:O	1:C:133:ILE:HG13	2.12	0.49
1:O:216:LEU:HB2	1:O:241:LYS:HZ1	1.73	0.49
1:O:280:THR:H	1:O:283:ASP:HB2	1.77	0.49
1:C:16:MET:O	1:C:17:ASP:HB2	2.13	0.49
1:C:322:LYS:HG2	1:C:323:PHE:CE1	2.48	0.49
1:C:73:LYS:HB3	1:C:94:GLN:CG	2.42	0.49
1:O:139:ARG:CA	1:O:139:ARG:HH21	2.26	0.49
1:O:35:VAL:HG21	1:O:128:VAL:HG21	1.95	0.49
1:C:216:LEU:CD2	1:C:216:LEU:N	2.75	0.49
1:C:256:VAL:HG23	1:C:297:THR:HA	1.94	0.49
1:O:139:ARG:HB2	1:O:139:ARG:CZ	2.43	0.49
1:C:111:VAL:HG13	1:C:113:GLU:O	2.12	0.48
1:C:144:PHE:CE1	1:C:148:ILE:HD11	2.47	0.48
1:C:295:LEU:HD23	1:C:295:LEU:HA	1.67	0.48
1:C:186:TYR:HA	1:C:338:LEU:O	2.13	0.48
1:O:216:LEU:CD1	1:O:241:LYS:HE2	2.43	0.48
1:C:193:ILE:CD1	1:C:203:ILE:HD12	2.43	0.48
1:C:258:LYS:HA	1:C:295:LEU:HD23	1.95	0.48
1:C:156:ASP:HB3	1:C:329:ARG:HB2	1.95	0.48
1:C:156:ASP:O	1:C:329:ARG:HB2	2.14	0.48
1:O:161:TYR:HE2	1:O:172:LEU:HD23	1.78	0.48
1:O:298:LEU:N	1:O:298:LEU:HD23	2.28	0.48
1:C:36:VAL:HG13	2:C:1341:C61:H2C2	1.95	0.48
1:C:306:PRO:C	1:C:308:PRO:HD2	2.34	0.48
1:C:133:ILE:HG22	1:C:134:GLU:OE1	2.13	0.48
1:O:216:LEU:HD23	1:O:217:CYS:N	2.24	0.48
1:C:104:VAL:HG11	1:C:147:ILE:HG13	1.95	0.48
1:O:152:VAL:HG12	1:O:153:LEU:N	2.28	0.48
1:O:155:GLU:O	1:O:157:VAL:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:224:LEU:O	1:O:314:ALA:HA	2.13	0.48
1:C:253:PHE:O	1:C:301:HIS:HE1	1.97	0.48
1:O:251:ARG:CG	1:O:252:LEU:N	2.75	0.48
1:C:200:VAL:HG12	1:C:202:GLN:HB2	1.93	0.48
1:C:258:LYS:HE3	1:C:261:GLU:OE1	2.14	0.48
1:O:88:VAL:HG13	1:O:119:PHE:CE2	2.49	0.48
1:O:306:PRO:C	1:O:308:PRO:HD2	2.33	0.48
1:C:79:LEU:CD2	1:C:92:LEU:HD21	2.30	0.48
1:O:196:ILE:O	1:O:196:ILE:HG23	2.13	0.48
1:O:257:VAL:HG21	1:O:265:LEU:HD11	1.94	0.48
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.45	0.47
1:O:275:LYS:HE2	1:O:275:LYS:HB2	1.28	0.47
1:O:115:PRO:C	1:O:117:LEU:N	2.67	0.47
1:O:216:LEU:HB2	1:O:241:LYS:CE	2.45	0.47
1:O:61:HIS:HD2	1:O:125:ASP:OD1	1.97	0.47
1:O:39:THR:HG23	1:O:227:THR:OG1	2.13	0.47
1:O:309:THR:CG2	1:O:310:GLY:N	2.77	0.47
1:C:260:ASN:HD22	1:C:261:GLU:CA	2.25	0.47
1:C:280:THR:HG21	1:O:23:GLU:OE2	2.14	0.47
1:C:205:MET:HE3	1:C:313:TRP:CD1	2.49	0.47
1:O:91:PHE:HE1	1:O:112:THR:HG23	1.80	0.47
2:O:1341:C61:H231	2:O:1341:C61:C16	2.27	0.47
1:O:150:GLN:HB3	1:O:152:VAL:HB	1.96	0.47
1:O:197:LYS:CB	1:O:197:LYS:NZ	2.77	0.47
1:O:251:ARG:HH12	1:O:253:PHE:CB	2.24	0.47
1:C:79:LEU:CD1	1:C:137:ILE:HG22	2.45	0.47
1:C:172:LEU:HD12	1:C:172:LEU:HA	1.48	0.47
1:O:237:SER:O	1:O:240:GLU:HB2	2.14	0.47
1:C:103:THR:O	1:C:103:THR:HG22	2.12	0.47
1:C:155:GLU:HB3	1:C:157:VAL:CG2	2.45	0.47
1:O:132:PHE:HB2	1:O:199:GLY:O	2.15	0.47
1:C:306:PRO:HB2	1:C:307:PRO:CD	2.44	0.47
1:O:148:ILE:HG13	1:O:156:ASP:OD2	2.14	0.47
1:O:53:ARG:HB2	1:O:59:VAL:CG2	2.44	0.47
1:C:130:MET:HE2	1:C:130:MET:HB3	1.82	0.47
1:C:217:CYS:O	1:C:217:CYS:SG	2.73	0.47
1:O:309:THR:HG22	1:O:310:GLY:H	1.78	0.47
1:O:227:THR:HG22	1:O:320:ILE:CD1	2.44	0.47
1:C:192:TYR:HA	1:C:334:ILE:O	2.16	0.46
1:O:115:PRO:O	1:O:118:PRO:HD2	2.16	0.46
1:C:200:VAL:HG12	1:C:200:VAL:O	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:PRO:CG	2:C:1341:C61:H13	2.45	0.46
1:O:5:ASN:CA	1:O:154:LYS:CE	2.92	0.46
1:O:214:THR:O	1:O:214:THR:HG23	2.14	0.46
1:O:88:VAL:CG1	1:O:119:PHE:CE2	2.98	0.46
1:C:5:ASN:C	1:C:5:ASN:ND2	2.68	0.46
1:O:97:ILE:HG22	1:O:98:THR:N	2.29	0.46
1:C:60:TYR:HB2	1:C:120:MET:CE	2.46	0.46
1:O:214:THR:CG2	1:O:218:GLU:HG3	2.43	0.46
1:C:249:LYS:N	1:C:249:LYS:HD3	2.31	0.46
1:C:81:LEU:O	1:C:87:THR:HA	2.15	0.46
1:O:236:THR:O	1:O:240:GLU:HG3	2.15	0.46
1:O:291:SER:CB	1:O:294:LYS:HD2	2.45	0.46
1:C:186:TYR:CE2	1:C:190:PHE:CE1	3.03	0.46
1:C:28:THR:HG1	1:C:71:SER:CB	2.24	0.46
1:C:60:TYR:HB2	1:C:120:MET:HE1	1.98	0.46
1:C:205:MET:HB3	1:C:205:MET:HE2	1.77	0.46
1:C:206:LYS:HB2	1:C:271:HIS:HD2	1.81	0.46
1:C:293:LYS:O	1:C:294:LYS:HG2	2.15	0.46
1:C:306:PRO:CB	1:C:307:PRO:CD	2.94	0.46
1:O:49:SER:C	1:O:51:CYS:H	2.19	0.46
1:O:251:ARG:NH1	1:O:253:PHE:HB2	2.25	0.45
1:C:198:THR:HB	1:C:332:ASN:HD22	1.80	0.45
1:O:118:PRO:HD2	1:O:119:PHE:H	1.80	0.45
1:O:309:THR:HG22	1:O:310:GLY:N	2.31	0.45
1:C:193:ILE:HG21	1:C:203:ILE:HG13	1.99	0.45
1:C:57:ALA:HA	1:C:120:MET:HE1	1.99	0.45
1:C:239:ILE:HG21	1:C:302:ALA:HB2	1.97	0.45
1:O:153:LEU:C	1:O:154:LYS:HE2	2.37	0.45
1:O:49:SER:C	1:O:51:CYS:N	2.70	0.45
1:C:127:VAL:HG12	1:C:127:VAL:O	2.17	0.45
1:C:54:LEU:HA	1:C:54:LEU:HD12	1.68	0.45
1:O:119:PHE:C	1:O:121:LEU:N	2.69	0.45
1:O:213:SER:O	1:O:215:LEU:HD23	2.17	0.45
1:O:216:LEU:CD2	1:O:217:CYS:N	2.79	0.45
1:O:307:PRO:HA	1:O:310:GLY:O	2.17	0.45
1:O:6:THR:CG2	1:O:7:THR:N	2.78	0.45
1:C:9:SER:HA	1:C:176:ILE:O	2.17	0.45
1:C:280:THR:O	1:C:283:ASP:HB2	2.17	0.45
1:C:57:ALA:HB1	1:C:114:MET:HG2	1.98	0.45
1:C:242:LEU:CD1	1:C:242:LEU:C	2.85	0.45
1:C:157:VAL:HG12	1:C:327:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:CE2	2:C:1341:C61:H203	2.52	0.45
1:C:175:GLN:HE21	1:C:175:GLN:HB3	1.35	0.45
1:C:193:ILE:HD13	1:C:203:ILE:HD12	1.99	0.45
1:O:306:PRO:HA	1:O:307:PRO:HD3	1.62	0.45
1:C:20:TYR:H	2:C:1341:C61:H2C1	1.82	0.44
1:C:242:LEU:HD12	1:C:242:LEU:C	2.37	0.44
1:O:24:ILE:HG12	1:O:35:VAL:CG1	2.47	0.44
1:C:83:TYR:CD2	2:C:1341:C61:C20	3.01	0.44
1:O:211:GLY:HA2	1:O:266:PRO:HB3	1.99	0.44
1:O:75:ASN:OD1	1:O:77:THR:HG22	2.17	0.44
1:C:6:THR:OG1	1:C:152:VAL:HG23	2.17	0.44
1:O:121:LEU:HD23	1:O:121:LEU:HA	1.57	0.44
1:O:259:CYS:HB3	1:O:289:SER:O	2.18	0.44
1:O:305:ILE:HA	1:O:306:PRO:HD3	1.62	0.44
1:C:115:PRO:O	1:C:119:PHE:HB2	2.18	0.44
1:C:19:GLN:NE2	1:C:123:GLU:HB2	2.32	0.44
1:O:215:LEU:N	1:O:215:LEU:HD23	2.33	0.44
1:C:214:THR:CG2	1:C:218:GLU:HB3	2.47	0.44
1:O:6:THR:HB	1:O:152:VAL:O	2.17	0.44
1:O:220:GLY:O	1:O:221:CYS:HB3	2.17	0.44
1:C:94:GLN:HB3	1:C:107:MET:HE2	2.00	0.44
1:O:181:SER:O	1:O:183:PRO:HD3	2.18	0.43
1:O:197:LYS:HB2	1:O:197:LYS:NZ	2.32	0.43
1:O:280:THR:N	1:O:283:ASP:HB2	2.33	0.43
1:C:154:LYS:NZ	1:C:154:LYS:CB	2.71	0.43
1:O:260:ASN:HB2	1:O:292:SER:CA	2.47	0.43
1:O:88:VAL:HG12	1:O:115:PRO:CD	2.48	0.43
1:C:239:ILE:HD13	1:C:239:ILE:HA	1.33	0.43
1:C:260:ASN:HD21	1:C:261:GLU:HG3	1.82	0.43
1:O:252:LEU:HB3	1:O:253:PHE:CD1	2.53	0.43
1:O:205:MET:HE3	1:O:270:PHE:HD2	1.80	0.43
1:O:306:PRO:CB	1:O:307:PRO:HD2	2.48	0.43
1:C:225:VAL:HG21	1:C:334:ILE:HD13	2.01	0.43
1:C:333:ARG:H	1:C:333:ARG:HG3	1.49	0.43
2:O:1341:C61:H231	2:O:1341:C61:H162	1.82	0.43
1:O:192:TYR:N	1:O:192:TYR:CD1	2.86	0.43
1:O:197:LYS:HB2	1:O:197:LYS:HZ2	1.84	0.43
1:C:111:VAL:HG13	1:C:113:GLU:H	1.84	0.43
1:C:287:GLN:HE21	1:C:287:GLN:HB2	1.59	0.43
1:O:118:PRO:HG2	1:O:119:PHE:CE2	2.51	0.43
1:O:305:ILE:C	1:O:310:GLY:HA3	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:TYR:HB2	1:C:95:ASP:OD2	2.19	0.43
1:O:24:ILE:HD12	1:O:97:ILE:HG23	2.01	0.43
1:O:251:ARG:NH2	1:O:254:ASP:HB2	2.33	0.43
1:O:99:VAL:O	1:O:102:ILE:HB	2.19	0.43
1:C:97:ILE:CG2	1:C:98:THR:N	2.82	0.42
1:O:104:VAL:HG21	1:O:143:ILE:HD11	2.01	0.42
1:C:215:LEU:HB3	1:C:216:LEU:CD2	2.48	0.42
1:O:176:ILE:HD13	1:O:176:ILE:HG23	1.62	0.42
1:C:242:LEU:CD1	1:C:246:LEU:CD1	2.97	0.42
1:O:66:ALA:HB1	1:O:72:TYR:CD2	2.54	0.42
1:C:16:MET:C	1:C:18:THR:N	2.71	0.42
1:C:206:LYS:NZ	1:C:274:GLY:H	2.18	0.42
1:O:281:SER:O	1:O:285:VAL:HB	2.19	0.42
1:O:39:THR:HG22	1:O:130:MET:HB2	2.01	0.42
1:C:104:VAL:O	1:C:104:VAL:HG23	2.16	0.42
1:C:307:PRO:N	1:C:308:PRO:HD2	2.35	0.42
1:C:84:SER:HB2	2:C:1341:C61:C26	2.41	0.42
1:O:96:ILE:HD13	1:O:96:ILE:HG21	1.80	0.42
1:C:27:GLY:O	1:C:30:PRO:HA	2.19	0.42
1:C:192:TYR:CD2	1:C:335:GLY:CA	3.03	0.42
1:O:103:THR:HG23	1:O:103:THR:O	2.20	0.42
1:O:340:ARG:NH2	1:O:340:ARG:CG	2.81	0.42
1:O:230:SER:O	1:O:317:ALA:HB3	2.20	0.42
1:O:271:HIS:HB2	1:O:276:GLU:CD	2.40	0.42
1:O:215:LEU:HB2	1:O:241:LYS:NZ	2.34	0.41
1:C:155:GLU:O	1:C:179:GLY:HA2	2.20	0.41
1:O:153:LEU:HA	1:O:153:LEU:HD23	1.80	0.41
1:O:205:MET:HE3	1:O:208:VAL:HG22	2.00	0.41
1:O:260:ASN:O	1:O:263:PRO:HD2	2.20	0.41
1:O:34:LYS:O	1:O:125:ASP:N	2.50	0.41
1:O:141:THR:HG22	1:O:142:PRO:N	2.34	0.41
1:C:83:TYR:CZ	2:C:1341:C61:H203	2.55	0.41
1:O:36:VAL:HG11	2:O:1341:C61:H5C1	2.02	0.41
1:O:96:ILE:HA	1:O:104:VAL:O	2.20	0.41
1:C:200:VAL:HG12	1:C:202:GLN:N	2.35	0.41
1:C:153:LEU:HD22	1:C:179:GLY:CA	2.49	0.41
1:C:19:GLN:CG	2:C:1341:C61:H5C1	2.51	0.41
1:O:281:SER:O	1:O:282:ALA:O	2.38	0.41
1:O:45:TRP:CE3	1:O:111:VAL:CG2	3.02	0.41
1:O:47:PRO:HG2	1:O:62:LYS:O	2.20	0.41
1:C:64:PHE:HE1	1:C:66:ALA:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:17:ASP:O	1:O:321:ARG:NH2	2.53	0.41
1:C:200:VAL:HG12	1:C:202:GLN:H	1.86	0.41
1:O:5:ASN:C	1:O:154:LYS:HE3	2.39	0.41
1:C:47:PRO:CG	1:C:114:MET:CE	2.98	0.41
1:C:132:PHE:CD2	1:C:199:GLY:C	2.95	0.41
1:O:16:MET:C	1:O:18:THR:H	2.23	0.41
1:O:328:ASP:HB3	1:O:333:ARG:O	2.21	0.41
1:O:340:ARG:HH21	1:O:340:ARG:CB	2.34	0.41
1:C:193:ILE:CD1	1:C:203:ILE:CD1	2.99	0.41
1:O:195:LEU:HD12	1:O:195:LEU:HA	1.69	0.41
2:C:1341:C61:H161	2:C:1341:C61:H202	1.79	0.40
1:O:214:THR:CG2	1:O:214:THR:O	2.68	0.40
1:O:27:GLY:HA2	1:O:95:ASP:OD1	2.21	0.40
1:O:234:GLY:H	1:O:302:ALA:HA	1.86	0.40
1:O:65:ASP:O	1:O:67:SER:N	2.53	0.40
1:C:265:LEU:HD23	1:C:284:TYR:HE1	1.86	0.40
1:O:118:PRO:CD	1:O:119:PHE:N	2.83	0.40
1:O:216:LEU:CD1	1:O:241:LYS:CE	2.99	0.40
1:O:215:LEU:CB	1:O:241:LYS:NZ	2.84	0.40
1:O:72:TYR:OH	1:O:74:HIS:HA	2.21	0.40
1:C:200:VAL:HG12	1:C:202:GLN:CB	2.51	0.40
1:C:258:LYS:HE3	1:C:258:LYS:HB2	1.92	0.40
1:O:280:THR:O	1:O:284:TYR:CD2	2.74	0.40
1:C:155:GLU:O	1:C:157:VAL:N	2.53	0.40
1:C:263:PRO:HG3	1:C:290:TYR:CD2	2.57	0.40
1:C:286:PHE:O	1:C:288:GLU:OE1	2.39	0.40
1:O:144:PHE:CE1	1:O:148:ILE:HG12	2.56	0.40
1:C:216:LEU:HA	1:C:218:GLU:OE1	2.21	0.40
1:C:310:GLY:HA2	1:C:312:THR:HB	2.03	0.40
1:O:251:ARG:NH1	1:O:253:PHE:C	2.75	0.40
1:O:300:ILE:C	1:O:301:HIS:CD2	2.94	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%)	288 (87%)	31 (9%)	11 (3%)	4	25
1	O	328/340 (96%)	281 (86%)	30 (9%)	17 (5%)	2	14
All	All	658/680 (97%)	569 (86%)	61 (9%)	28 (4%)	3	18

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	196	ILE
1	C	218	GLU
1	C	251	ARG
1	C	252	LEU
1	O	66	ALA
1	O	85	THR
1	O	156	ASP
1	O	165	ASP
1	O	220	GLY
1	O	254	ASP
1	O	307	PRO
1	C	152	VAL
1	C	214	THR
1	C	245	ALA
1	C	262	GLY
1	C	307	PRO
1	O	68	ASP
1	O	95	ASP
1	O	197	LYS
1	O	214	THR
1	C	151	GLY
1	O	76	GLY
1	O	283	ASP
1	O	289	SER
1	O	282	ALA
1	C	308	PRO
1	O	266	PRO
1	O	308	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	C	283/290 (98%)	222 (78%)	61 (22%)	1	5
1	O	282/290 (97%)	201 (71%)	81 (29%)	0	1
All	All	565/580 (97%)	423 (75%)	142 (25%)	0	2

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	ASN
1	C	9	SER
1	C	11	ILE
1	C	26	ILE
1	C	32	THR
1	C	48	SER
1	C	53	ARG
1	C	62	LYS
1	C	63	LEU
1	C	68	ASP
1	C	84	SER
1	C	89	SER
1	C	113	GLU
1	C	117	LEU
1	C	130	MET
1	C	137	ILE
1	C	143	ILE
1	C	145	ASP
1	C	152	VAL
1	C	154	LYS
1	C	157	VAL
1	C	164	ARG
1	C	165	ASP
1	C	175	GLN
1	C	195	LEU
1	C	198	THR
1	C	203	ILE

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Mol	Chain	Res	Type
1	C	204	GLN
1	C	206	LYS
1	C	213	SER
1	C	216	LEU
1	C	218	GLU
1	C	224	LEU
1	C	230	SER
1	C	237	SER
1	C	238	SER
1	C	239	ILE
1	C	240	GLU
1	C	241	LYS
1	C	242	LEU
1	C	244	GLU
1	C	250	LYS
1	C	251	ARG
1	C	252	LEU
1	C	256	VAL
1	C	257	VAL
1	C	259	CYS
1	C	260	ASN
1	C	288	GLU
1	C	289	SER
1	C	291	SER
1	C	294	LYS
1	C	298	LEU
1	C	309	THR
1	C	318	THR
1	C	321	ARG
1	C	329	ARG
1	C	330	ARG
1	C	333	ARG
1	C	338	LEU
1	C	340	ARG
1	O	5	ASN
1	O	7	THR
1	O	8	SER
1	O	9	SER
1	O	20	TYR
1	O	23	GLU
1	O	28	THR
1	O	29	PRO

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Mol	Chain	Res	Type
1	O	31	GLN
1	O	32	THR
1	O	38	ASP
1	O	41	SER
1	O	42	SER
1	O	50	LYS
1	O	52	SER
1	O	53	ARG
1	O	56	THR
1	O	62	LYS
1	O	70	SER
1	O	73	LYS
1	O	77	THR
1	O	79	LEU
1	O	92	LEU
1	O	93	SER
1	O	95	ASP
1	O	98	THR
1	O	113	GLU
1	O	114	MET
1	O	117	LEU
1	O	125	ASP
1	O	133	ILE
1	O	139	ARG
1	O	148	ILE
1	O	150	GLN
1	O	154	LYS
1	O	157	VAL
1	O	159	SER
1	O	163	ASN
1	O	165	ASP
1	O	171	SER
1	O	172	LEU
1	O	175	GLN
1	O	176	ILE
1	O	182	ASP
1	O	189	ASN
1	O	196	ILE
1	O	197	LYS
1	O	200	VAL
1	O	206	LYS
1	O	212	SER

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Mol	Chain	Res	Type
1	O	214	THR
1	O	216	LEU
1	O	224	LEU
1	O	230	SER
1	O	238	SER
1	O	241	LYS
1	O	243	MET
1	O	244	GLU
1	O	246	LEU
1	O	249	LYS
1	O	251	ARG
1	O	252	LEU
1	O	254	ASP
1	O	257	VAL
1	O	258	LYS
1	O	272	LEU
1	O	275	LYS
1	O	278	THR
1	O	280	THR
1	O	287	GLN
1	O	288	GLU
1	O	291	SER
1	O	295	LEU
1	O	297	THR
1	O	303	MET
1	O	305	ILE
1	O	309	THR
1	O	322	LYS
1	O	329	ARG
1	O	338	LEU
1	O	340	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	5	ASN
1	C	19	GLN
1	C	175	GLN
1	C	189	ASN
1	C	260	ASN
1	C	287	GLN
1	C	301	HIS

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Mol	Chain	Res	Type
1	C	332	ASN
1	O	61	HIS
1	O	106	GLN
1	O	175	GLN
1	O	189	ASN
1	O	191	HIS
1	O	202	GLN
1	O	287	GLN
1	O	301	HIS
1	O	332	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	C61	C	1341	-	34,34,34	1.44	4 (11%)	37,43,43	1.84	8 (21%)
2	C61	O	1341	-	34,34,34	1.13	3 (8%)	37,43,43	2.18	8 (21%)

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	C61	C	1341	-	-	0/37/37/37	0/1/1/1
2	C61	O	1341	-	-	0/37/37/37	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1341	C61	C19-C18	-4.13	1.37	1.52
2	O	1341	C61	C14-C13	2.24	1.42	1.38
2	C	1341	C61	C28-C27	2.48	1.61	1.52
2	O	1341	C61	O7-C11	3.26	1.44	1.37
2	C	1341	C61	O7-C11	3.35	1.44	1.37
2	O	1341	C61	O8-C12	4.01	1.43	1.37
2	C	1341	C61	O8-C12	4.31	1.43	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1341	C61	C27-C26-C24	-5.72	106.81	114.32
2	O	1341	C61	C27-C26-C24	-5.29	107.38	114.32
2	O	1341	C61	C6-O7-C11	-3.91	108.17	117.70
2	C	1341	C61	C15-C16-C17	-3.59	107.66	113.77
2	C	1341	C61	C6-O7-C11	-3.29	109.69	117.70
2	O	1341	C61	C15-C16-C17	-3.18	108.37	113.77
2	C	1341	C61	O8-C12-C13	-2.54	120.10	124.37
2	O	1341	C61	O7-C11-C10	-2.37	117.85	123.61
2	O	1341	C61	O8-C12-C13	-2.21	120.65	124.37
2	C	1341	C61	C33-C32-N31	2.15	118.37	112.18
2	C	1341	C61	O7-C11-C12	2.29	120.54	115.76
2	O	1341	C61	O7-C11-C12	2.40	120.77	115.76
2	O	1341	C61	O8-C12-C11	2.97	119.48	115.41
2	C	1341	C61	O8-C12-C11	3.66	120.43	115.41
2	C	1341	C61	C9-O8-C12	4.20	123.58	117.54
2	O	1341	C61	C9-O8-C12	8.87	130.30	117.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1341	C61	22	0
2	O	1341	C61	9	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.