



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:36 pm BST

PDB ID : 2RUS  
Title : CRYSTAL STRUCTURE OF THE TERNARY COMPLEX OF RIBULOSE  
-1,5-BISPHOSPHATE CARBOXYLASE, MG(II), AND ACTIVATOR CO2  
AT 2.3-ANGSTROMS RESOLUTION  
Authors : Lundqvist, T.; Schneider, G.  
Deposited on : 1991-10-11  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

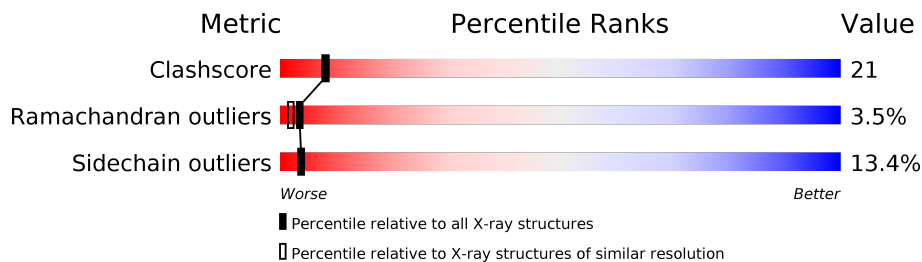
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	490	
1	B	490	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7447 atoms, of which 2 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 RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3339	2115	590	619	15	14	0	0
1	B	444	3386	2145	598	627	16	28	0	0

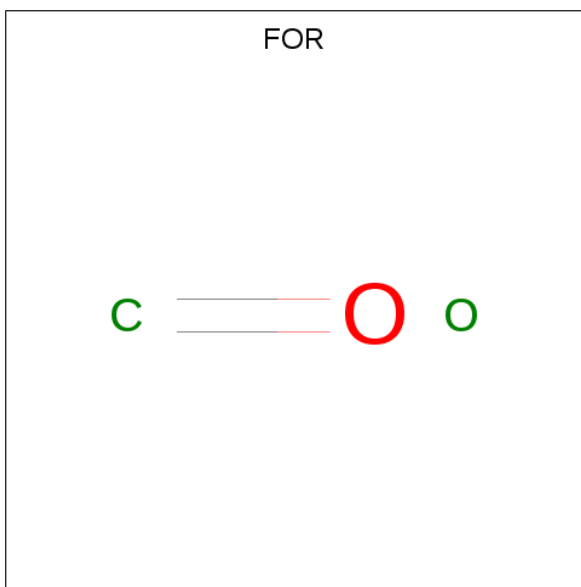
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	CONFLICT	UNP P04718
B	91	ASP	HIS	CONFLICT	UNP P04718

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	B	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is FORMYL GROUP (three-letter code: FOR) (formula: CH<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			3	1	1	1		
3	B	1	Total	C	H	O	0	0
			3	1	1	1		

- Molecule 4 is water.

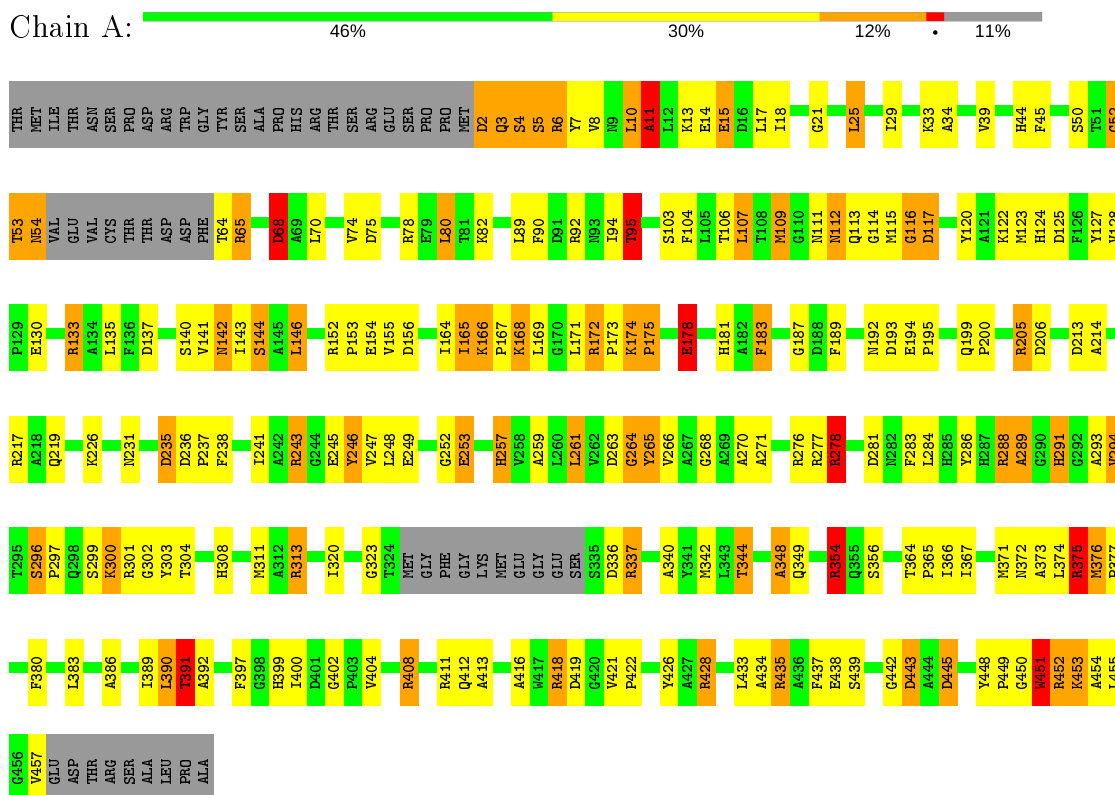
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	340	Total	O	0	0
			340	340		
4	B	374	Total	O	0	0
			374	374		

### 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. 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: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.50Å 70.60Å 104.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	5.50 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (5.50-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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: MG, FOR

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	0.85	0/3419	2.07	105/4633 (2.3%)
1	B	0.87	0/3467	1.97	102/4694 (2.2%)
All	All	0.86	0/6886	2.02	207/9327 (2.2%)

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	A	0	2

There are no bond length outliers.

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	CD-NE-CZ	35.46	173.25	123.60
1	B	375	ARG	CD-NE-CZ	22.46	155.04	123.60
1	A	277	ARG	NE-CZ-NH1	16.84	128.72	120.30
1	A	205	ARG	NE-CZ-NH2	16.59	128.60	120.30
1	A	435	ARG	NE-CZ-NH1	16.35	128.48	120.30
1	A	313	ARG	NE-CZ-NH2	14.00	127.30	120.30
1	A	205	ARG	NE-CZ-NH1	-13.18	113.71	120.30
1	B	408	ARG	NE-CZ-NH2	-12.79	113.91	120.30
1	A	6	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	B	337	ARG	CD-NE-CZ	11.66	139.92	123.60
1	B	133	ARG	CD-NE-CZ	11.47	139.66	123.60
1	B	172	ARG	CG-CD-NE	11.12	135.15	111.80
1	A	92	ARG	NE-CZ-NH1	-11.07	114.77	120.30
1	B	337	ARG	NE-CZ-NH1	10.98	125.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	ARG	CD-NE-CZ	10.63	138.48	123.60
1	A	133	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	B	235	ASP	CB-CG-OD1	-10.46	108.89	118.30
1	A	172	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	B	165	ILE	N-CA-CB	-10.40	86.87	110.80
1	B	336	ASP	CB-CG-OD1	10.20	127.48	118.30
1	B	172	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	B	328	GLY	O-C-N	10.02	138.73	122.70
1	A	127	TYR	CB-CG-CD2	-9.75	115.15	121.00
1	A	263	ASP	C-N-CA	9.73	142.72	122.30
1	B	457	VAL	CA-C-O	-9.62	99.90	120.10
1	A	127	TYR	CB-CG-CD1	9.29	126.57	121.00
1	B	188	ASP	CB-CG-OD1	9.23	126.61	118.30
1	A	419	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	B	277	ARG	NE-CZ-NH1	-9.08	115.76	120.30
1	A	172	ARG	NE-CZ-NH1	8.99	124.79	120.30
1	A	137	ASP	CB-CG-OD1	8.87	126.28	118.30
1	B	204	LEU	CA-CB-CG	8.57	135.02	115.30
1	A	418	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	A	95	THR	CA-CB-CG2	8.40	124.16	112.40
1	A	408	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	B	78	ARG	NE-CZ-NH1	-8.27	116.17	120.30
1	B	206	ASP	CB-CG-OD1	8.26	125.73	118.30
1	A	205	ARG	CD-NE-CZ	8.25	135.14	123.60
1	B	213	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	A	137	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	B	426	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	B	109	MET	N-CA-CB	-8.10	96.03	110.60
1	A	3	GLN	CA-C-O	8.03	136.96	120.10
1	A	78	ARG	NE-CZ-NH2	7.95	124.27	120.30
1	A	435	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	245	GLU	CA-CB-CG	7.78	130.52	113.40
1	A	337	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	227	LEU	CA-CB-CG	7.77	133.16	115.30
1	B	236	ASP	CB-CG-OD1	7.76	125.29	118.30
1	A	235	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	B	428	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	291	HIS	C-N-CA	7.66	138.38	122.30
1	B	411	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	A	92	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	A	116	GLY	N-CA-C	-7.33	94.78	113.10
1	A	313	ARG	NH1-CZ-NH2	-7.31	111.36	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	ARG	CD-NE-CZ	7.30	133.82	123.60
1	A	303	TYR	CB-CG-CD2	-7.26	116.65	121.00
1	A	109	MET	CA-CB-CG	7.18	125.51	113.30
1	A	313	ARG	CG-CD-NE	7.13	126.78	111.80
1	B	443	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	408	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	428	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	224	GLU	OE1-CD-OE2	7.02	131.72	123.30
1	A	452	ARG	CD-NE-CZ	7.01	133.41	123.60
1	B	418	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	127	TYR	CB-CG-CD1	-6.97	116.82	121.00
1	B	205	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	125	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	278	ARG	NE-CZ-NH1	-6.81	116.90	120.30
1	B	328	GLY	CA-C-O	-6.80	108.37	120.60
1	B	354	ARG	CD-NE-CZ	6.79	133.11	123.60
1	A	25	LEU	CB-CA-C	6.79	123.10	110.20
1	A	217	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	B	410	LEU	CA-CB-CG	6.76	130.85	115.30
1	A	14	GLU	OE1-CD-OE2	-6.71	115.24	123.30
1	B	206	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	193	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	445	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	65	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	B	419	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	B	172	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	75	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	109	MET	N-CA-CB	-6.61	98.71	110.60
1	B	305	ALA	CB-CA-C	6.59	119.98	110.10
1	A	265	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	A	278	ARG	CD-NE-CZ	6.56	132.79	123.60
1	B	5	SER	C-N-CA	6.48	137.90	121.70
1	A	263	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	154	GLU	CA-CB-CG	6.42	127.52	113.40
1	B	276	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	B	363	CYS	CB-CA-C	6.36	123.11	110.40
1	A	11	ALA	N-CA-CB	6.35	118.99	110.10
1	B	382	ASN	CA-CB-CG	-6.32	99.49	113.40
1	A	3	GLN	N-CA-CB	6.32	121.97	110.60
1	B	213	ASP	OD1-CG-OD2	6.29	135.25	123.30
1	B	408	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	264	GLY	N-CA-C	6.28	128.80	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	TRP	CA-CB-CG	6.27	125.61	113.70
1	A	10	LEU	N-CA-C	-6.21	94.25	111.00
1	B	346	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	A	213	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	178	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	B	74	VAL	CB-CA-C	6.13	123.05	111.40
1	B	303	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	206	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	4	SER	N-CA-C	-6.12	94.47	111.00
1	B	72	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	A	259	ALA	N-CA-CB	6.09	118.63	110.10
1	A	303	TYR	CB-CG-CD1	6.09	124.66	121.00
1	A	386	ALA	C-N-CA	6.09	136.92	121.70
1	A	78	ARG	CD-NE-CZ	6.08	132.11	123.60
1	A	189	PHE	N-CA-CB	-6.07	99.67	110.60
1	A	10	LEU	CA-C-O	-6.06	107.38	120.10
1	A	154	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	B	216	ARG	CD-NE-CZ	-6.03	115.16	123.60
1	B	133	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	B	304	THR	N-CA-CB	-6.03	98.85	110.30
1	B	346	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	72	TYR	CB-CG-CD2	6.00	124.60	121.00
1	B	401	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	301	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	A	140	SER	N-CA-CB	5.96	119.44	110.50
1	B	36	TYR	CA-CB-CG	5.96	124.72	113.40
1	B	194	GLU	CA-CB-CG	5.95	126.49	113.40
1	B	165	ILE	CB-CA-C	5.92	123.44	111.60
1	A	277	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	100	MET	CG-SD-CE	-5.87	90.81	100.20
1	B	3	GLN	C-N-CA	5.84	136.31	121.70
1	A	301	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	B	290	GLY	C-N-CA	5.83	136.27	121.70
1	A	144	SER	N-CA-CB	5.82	119.23	110.50
1	A	193	ASP	OD1-CG-OD2	-5.81	112.27	123.30
1	B	418	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	288	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	344	THR	N-CA-CB	-5.73	99.41	110.30
1	A	165	ILE	O-C-N	5.71	131.84	122.70
1	B	375	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	A	386	ALA	N-CA-CB	-5.69	102.13	110.10
1	A	296	SER	N-CA-CB	5.67	119.01	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	154	GLU	CG-CD-OE2	-5.65	107.01	118.30
1	A	39	VAL	CB-CA-C	5.62	122.07	111.40
1	B	67	VAL	CA-CB-CG1	5.62	119.32	110.90
1	A	245	GLU	CG-CD-OE1	5.61	129.52	118.30
1	A	90	PHE	CB-CA-C	5.60	121.60	110.40
1	B	372	ASN	CA-CB-CG	5.59	125.71	113.40
1	B	445	ASP	CA-CB-CG	5.59	125.71	113.40
1	B	172	ARG	CB-CA-C	5.57	121.55	110.40
1	B	343	LEU	CA-CB-CG	5.57	128.12	115.30
1	A	94	ILE	C-N-CA	5.56	135.61	121.70
1	B	28	TYR	CB-CA-C	-5.56	99.29	110.40
1	B	367	ILE	CB-CA-C	5.54	122.69	111.60
1	B	337	ARG	N-CA-CB	5.53	120.55	110.60
1	B	428	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	A	354	ARG	N-CA-CB	5.50	120.49	110.60
1	B	288	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	164	ILE	N-CA-CB	5.47	123.39	110.80
1	B	337	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	80	LEU	CB-CA-C	5.46	120.57	110.20
1	A	249	GLU	OE1-CD-OE2	5.44	129.83	123.30
1	B	67	VAL	CB-CA-C	5.42	121.70	111.40
1	A	288	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	354	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	205	ARG	CD-NE-CZ	-5.38	116.06	123.60
1	B	152	ARG	CD-NE-CZ	-5.37	116.08	123.60
1	A	375	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	69	ALA	CB-CA-C	5.33	118.09	110.10
1	B	316	GLY	CA-C-O	-5.33	111.01	120.60
1	A	144	SER	CB-CA-C	-5.33	99.98	110.10
1	A	257	HIS	O-C-N	5.30	131.19	122.70
1	B	383	LEU	CB-CA-C	5.29	120.25	110.20
1	B	376	MET	CA-CB-CG	5.29	122.28	113.30
1	A	3	GLN	CA-C-N	-5.28	105.58	117.20
1	B	337	ARG	CB-CG-CD	5.27	125.31	111.60
1	A	313	ARG	CA-CB-CG	5.26	124.97	113.40
1	B	426	TYR	CB-CG-CD1	5.26	124.16	121.00
1	B	127	TYR	CB-CG-CD2	5.25	124.15	121.00
1	B	347	GLU	OE1-CD-OE2	5.25	129.60	123.30
1	A	142	ASN	CB-CA-C	5.24	120.89	110.40
1	A	68	ASP	CA-CB-CG	5.24	124.93	113.40
1	A	263	ASP	N-CA-CB	5.20	119.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	SER	CB-CA-C	-5.20	100.22	110.10
1	B	245	GLU	CG-CD-OE2	-5.18	107.93	118.30
1	A	245	GLU	CG-CD-OE2	-5.18	107.94	118.30
1	A	445	ASP	CA-CB-CG	5.18	124.79	113.40
1	A	348	ALA	CB-CA-C	5.17	117.85	110.10
1	B	76	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	354	ARG	CA-CB-CG	5.15	124.73	113.40
1	B	115	MET	N-CA-C	5.14	124.89	111.00
1	A	146	LEU	CB-CA-C	5.13	119.96	110.20
1	B	174	LYS	CA-CB-CG	5.12	124.67	113.40
1	B	85	TYR	CB-CG-CD1	5.10	124.06	121.00
1	A	183	PHE	N-CA-CB	5.09	119.76	110.60
1	A	141	VAL	O-C-N	5.09	130.84	122.70
1	A	2	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	29	ILE	N-CA-C	-5.08	97.28	111.00
1	A	391	THR	CA-CB-CG2	5.07	119.50	112.40
1	A	435	ARG	CB-CA-C	5.06	120.52	110.40
1	A	246	TYR	CB-CG-CD1	5.05	124.03	121.00
1	A	304	THR	CA-CB-CG2	5.05	119.47	112.40
1	B	152	ARG	CA-CB-CG	-5.04	102.31	113.40
1	B	253	GLU	CA-CB-CG	5.03	124.46	113.40
1	B	277	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	A	15	GLU	CG-CD-OE2	-5.01	108.28	118.30
1	A	243	ARG	CD-NE-CZ	5.01	130.61	123.60
1	A	3	GLN	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	GLY	Mainchain
1	A	64	THR	Mainchain

## 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	3339	0	3238	140	0
1	B	3386	0	3285	155	6
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	1	0	0	0
3	B	2	1	0	0	0
4	A	340	0	0	13	6
4	B	374	0	0	13	10
All	All	7445	2	6523	282	13

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (282) 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:53:THR:O	1:A:54:ASN:HB2	1.47	1.07
1:A:219:GLN:HE21	1:A:226:LYS:H	1.02	1.01
1:A:438:GLU:OE2	1:A:457:VAL:HG22	1.64	0.98
1:B:333:GLU:HG2	1:B:334:SER:H	1.29	0.96
1:B:48:GLU:HB3	1:B:115:MET:HE1	1.48	0.94
1:A:174:LYS:HB3	1:A:175:PRO:HD3	1.50	0.94
1:B:304:THR:HG22	1:B:307:VAL:H	1.33	0.92
1:B:333:GLU:HG2	1:B:334:SER:N	1.87	0.90
1:B:272:ILE:HG21	1:B:315:GLN:HE21	1.40	0.85
1:A:52:GLY:O	1:A:53:THR:HB	1.74	0.84
1:A:53:THR:O	1:A:54:ASN:CB	2.23	0.83
1:B:335:SER:O	1:B:336:ASP:HB2	1.76	0.83
1:B:376:MET:HB3	1:B:377:PRO:HD3	1.60	0.82
1:A:146:LEU:HG	4:A:524:HOH:O	1.79	0.82
1:A:438:GLU:OE2	1:A:457:VAL:CG2	2.26	0.82
1:B:322:THR:HG22	1:B:323:GLY:H	1.44	0.81
1:B:337:ARG:HD3	1:B:337:ARG:O	1.80	0.81
1:B:151:GLY:HA2	4:B:753:HOH:O	1.82	0.78
1:B:152:ARG:HB3	1:B:153:PRO:HD2	1.65	0.77
1:A:8:VAL:HG13	1:A:10:LEU:HD13	1.67	0.76
1:A:428:ARG:HE	1:A:455:LEU:HA	1.52	0.73
1:B:194:GLU:HG2	1:B:195:PRO:HD3	1.71	0.72
1:A:168:LYS:HG2	1:B:50:SER:O	1.90	0.72
1:B:288:ARG:HH12	1:B:305:ALA:HB1	1.55	0.72
1:A:130:GLU:OE2	1:A:133:ARG:NH1	2.23	0.71
1:B:67:VAL:HG13	1:B:89:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:TYR:CE1	1:B:47:ALA:HA	2.27	0.69
1:B:181:HIS:HB2	1:B:214:ALA:HB1	1.74	0.69
1:A:80:LEU:HD11	1:A:82:LYS:HE3	1.75	0.69
1:A:65:ARG:HA	1:A:68:ASP:OD2	1.92	0.69
1:B:152:ARG:HG2	4:B:528:HOH:O	1.92	0.68
1:B:321:HIS:CE1	1:B:324:THR:HG23	2.29	0.68
1:B:67:VAL:O	1:B:89:LEU:HD11	1.95	0.67
1:A:116:GLY:O	1:A:117:ASP:HB2	1.94	0.67
1:B:272:ILE:HG21	1:B:315:GLN:NE2	2.09	0.67
1:A:219:GLN:NE2	1:A:226:LYS:H	1.84	0.67
1:A:400:ILE:HD12	1:A:435:ARG:HH11	1.59	0.66
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.76	0.66
1:B:183:PHE:HB3	1:B:190:ILE:HD11	1.77	0.66
1:A:455:LEU:C	1:A:457:VAL:H	1.98	0.66
1:A:241:ILE:HD13	1:A:278:ARG:HG3	1.78	0.66
1:A:376:MET:HB3	1:A:377:PRO:HD3	1.78	0.66
1:B:112:ASN:HA	1:B:115:MET:HG3	1.78	0.65
1:A:146:LEU:HD11	1:A:283:PHE:CD1	2.32	0.65
1:A:172:ARG:HD3	4:A:548:HOH:O	1.96	0.65
1:A:411:ARG:NH1	4:A:556:HOH:O	2.30	0.65
1:B:165:ILE:HG21	1:B:176:PHE:CE2	2.33	0.64
1:B:26:CYS:HB3	1:B:123:MET:HE2	1.80	0.64
1:B:324:THR:O	1:B:325:MET:HB3	1.98	0.64
1:A:175:PRO:HG2	4:A:548:HOH:O	1.97	0.63
1:B:165:ILE:HG21	1:B:176:PHE:HE2	1.64	0.63
1:A:143:ILE:HA	1:A:146:LEU:HD13	1.79	0.63
1:B:164:ILE:CD1	1:B:191:LYS:HD3	2.29	0.63
1:A:270:ALA:HA	1:B:235:ASP:O	1.97	0.62
1:B:39:VAL:HG22	1:B:74:VAL:HG11	1.81	0.62
1:B:38:TYR:HE2	1:B:74:VAL:HG22	1.64	0.62
1:A:299:SER:HB2	1:B:301:ARG:NH1	2.15	0.62
1:A:219:GLN:HE21	1:A:226:LYS:N	1.87	0.61
1:A:442:GLY:O	1:A:443:ASP:HB2	1.99	0.61
1:A:95:THR:HB	1:B:239:GLU:OE1	1.99	0.61
1:A:231:ASN:HA	1:A:261:LEU:HB3	1.82	0.61
1:A:391:THR:HG21	4:A:834:HOH:O	2.00	0.61
1:B:52:GLY:O	1:B:53:THR:HB	2.01	0.61
1:A:103:SER:HA	1:A:106:THR:HG22	1.83	0.60
1:B:38:TYR:CE2	1:B:74:VAL:HG22	2.36	0.60
1:B:222:THR:CG2	1:B:224:GLU:HB2	2.31	0.60
1:B:100:MET:CE	1:B:102:ALA:HB3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:TYR:CZ	1:B:291:HIS:HA	2.36	0.60
1:B:45:PHE:CE2	1:B:112:ASN:HB2	2.37	0.60
1:B:456:GLY:O	1:B:457:VAL:HB	2.01	0.60
1:A:116:GLY:O	1:A:117:ASP:CB	2.49	0.60
1:B:288:ARG:HH21	1:B:308:HIS:HD2	1.47	0.60
1:A:50:SER:O	1:B:168:LYS:HD2	2.01	0.60
1:B:67:VAL:HG13	1:B:89:LEU:CD1	2.32	0.60
1:A:219:GLN:HE22	1:A:257:HIS:CE1	2.21	0.59
1:A:371:MET:SD	1:A:375:ARG:HB3	2.43	0.59
1:A:399:HIS:HB3	1:A:402:GLY:O	2.02	0.59
1:A:237:PRO:O	1:A:241:ILE:HG13	2.03	0.58
1:A:340:ALA:O	1:A:344:THR:HB	2.03	0.58
1:B:152:ARG:HB3	1:B:153:PRO:CD	2.33	0.58
1:B:164:ILE:HD12	1:B:191:LYS:HD3	1.86	0.58
1:B:411:ARG:HG3	4:B:699:HOH:O	2.04	0.57
1:A:278:ARG:HD3	4:A:699:HOH:O	2.04	0.57
1:B:326:GLY:O	1:B:327:PHE:HB2	2.03	0.57
1:B:21:GLY:HA2	4:B:541:HOH:O	2.04	0.57
1:A:434:ALA:O	1:A:437:PHE:HB2	2.04	0.57
1:A:8:VAL:CG1	1:A:10:LEU:HD13	2.35	0.57
1:B:165:ILE:CG2	1:B:176:PHE:HE2	2.18	0.57
1:A:392:ALA:HB3	1:A:397:PHE:CZ	2.40	0.57
1:A:167:PRO:HG2	1:A:171:LEU:HD13	1.85	0.57
1:A:174:LYS:HB3	1:A:175:PRO:CD	2.28	0.56
1:A:349:GLN:HE22	1:A:354:ARG:NE	2.03	0.56
1:A:371:MET:HB3	1:A:375:ARG:HB2	1.86	0.56
1:B:265:TYR:HB3	1:B:289:ALA:O	2.06	0.56
1:A:344:THR:HG21	4:A:676:HOH:O	2.05	0.56
1:A:367:ILE:HD12	1:A:390:LEU:HD23	1.88	0.56
1:A:354:ARG:CZ	1:A:354:ARG:HB3	2.36	0.55
1:B:112:ASN:ND2	4:B:873:HOH:O	2.31	0.55
1:A:241:ILE:CD1	1:A:278:ARG:HG3	2.35	0.55
1:B:398:GLY:HA3	4:B:733:HOH:O	2.05	0.55
1:A:299:SER:HB2	1:B:301:ARG:HH11	1.70	0.55
1:B:287:HIS:CE1	1:B:289:ALA:HB2	2.41	0.55
1:A:174:LYS:HE3	1:A:178:GLU:OE1	2.07	0.55
1:A:172:ARG:HB3	1:A:173:PRO:CD	2.36	0.55
1:A:18:ILE:HD11	4:A:626:HOH:O	2.06	0.55
1:B:295:THR:HG23	1:B:305:ALA:HB2	1.88	0.55
1:B:8:VAL:HG23	1:B:43:ALA:HB2	1.88	0.55
1:A:128:VAL:HG23	1:A:133:ARG:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:TRP:CD1	1:B:226:LYS:HB3	2.42	0.54
1:A:400:ILE:HG12	1:A:439:SER:OG	2.08	0.54
1:B:112:ASN:HB3	1:B:115:MET:HE3	1.89	0.54
1:A:194:GLU:HB2	1:A:195:PRO:HD3	1.90	0.54
1:B:113:GLN:OE1	1:B:301:ARG:HB3	2.08	0.53
1:B:323:GLY:HA3	4:B:842:HOH:O	2.08	0.53
1:B:222:THR:HG22	1:B:224:GLU:HB2	1.90	0.53
1:B:215:MET:O	1:B:219:GLN:HG3	2.09	0.52
1:A:293:ALA:HB2	1:B:113:GLN:OE1	2.08	0.52
1:B:152:ARG:NH1	1:B:159:LEU:O	2.42	0.52
1:A:337:ARG:HH21	1:A:337:ARG:HB2	1.73	0.52
1:A:288:ARG:HD2	1:A:320:ILE:HD11	1.92	0.52
1:B:124:HIS:O	1:B:125:ASP:HB2	2.10	0.52
1:B:52:GLY:O	1:B:53:THR:CB	2.58	0.52
1:B:29:ILE:HA	1:B:79:GLU:O	2.10	0.52
1:B:393:GLY:O	1:B:397:PHE:HB2	2.10	0.51
1:B:100:MET:HE3	1:B:102:ALA:HB3	1.93	0.51
1:B:304:THR:CG2	1:B:306:PHE:HB3	2.40	0.51
1:A:288:ARG:HE	1:A:308:HIS:CD2	2.29	0.51
1:A:107:LEU:HD13	1:B:195:PRO:HB3	1.93	0.51
1:B:333:GLU:CG	1:B:334:SER:N	2.67	0.51
1:B:109:MET:HE1	1:B:303:TYR:HB3	1.93	0.50
1:A:371:MET:HB3	1:A:375:ARG:CB	2.41	0.50
1:A:453:LYS:HD2	1:A:454:ALA:N	2.27	0.50
1:A:445:ASP:HB3	1:A:451:TRP:HE1	1.75	0.50
1:A:164:ILE:HD11	1:A:391:THR:HG23	1.93	0.50
1:B:176:PHE:HE1	1:B:211:VAL:HG21	1.77	0.50
1:B:411:ARG:HH21	1:B:412:GLN:HG2	1.75	0.50
1:A:372:ASN:OD1	1:A:374:LEU:HB2	2.11	0.50
1:B:168:LYS:HG3	1:B:193:ASP:OD1	2.12	0.50
1:A:412:GLN:HB3	1:A:433:LEU:HD22	1.94	0.50
1:B:367:ILE:HD12	1:B:379:PHE:CZ	2.47	0.50
1:A:235:ASP:O	1:B:270:ALA:HA	2.12	0.49
1:B:261:LEU:HD23	1:B:285:HIS:O	2.13	0.49
1:B:397:PHE:CD1	1:B:403:PRO:HG3	2.48	0.49
1:A:146:LEU:N	1:A:146:LEU:HD12	2.27	0.49
1:B:31:LYS:NZ	1:B:119:GLU:OE2	2.40	0.49
1:A:349:GLN:HE22	1:A:354:ARG:CZ	2.26	0.48
1:B:222:THR:HG21	1:B:226:LYS:CE	2.43	0.48
1:B:33:LYS:O	1:B:36:TYR:HD1	1.96	0.48
1:B:142:ASN:ND2	1:B:361:LYS:HG2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LYS:HB2	1:B:361:LYS:HZ3	1.78	0.48
1:A:152:ARG:HB3	1:A:153:PRO:HD2	1.95	0.48
1:A:65:ARG:O	1:A:65:ARG:HD2	2.13	0.48
1:B:294:VAL:HG13	1:B:302:GLY:HA3	1.94	0.48
1:A:167:PRO:CG	1:A:171:LEU:HD13	2.43	0.48
1:A:183:PHE:CE1	1:A:187:GLY:HA3	2.49	0.48
1:A:455:LEU:C	1:A:457:VAL:N	2.65	0.48
1:B:8:VAL:CG2	1:B:43:ALA:HB2	2.43	0.48
1:A:10:LEU:O	1:A:11:ALA:CB	2.62	0.48
1:A:120:TYR:HB2	1:A:300:LYS:O	2.13	0.48
1:A:265:TYR:CE1	1:A:291:HIS:HA	2.48	0.47
1:B:32:PRO:CB	1:B:41:THR:HG21	2.44	0.47
1:A:130:GLU:CD	1:A:133:ARG:HH12	2.16	0.47
1:A:13:LYS:HB3	1:A:15:GLU:OE1	2.14	0.47
1:A:52:GLY:O	1:A:53:THR:CB	2.56	0.47
1:B:288:ARG:HD2	1:B:288:ARG:HH21	1.53	0.47
1:B:292:GLY:O	1:B:296:SER:HB2	2.14	0.47
1:A:265:TYR:OH	1:A:294:VAL:HG22	2.15	0.47
1:B:180:CYS:HA	1:B:190:ILE:HD13	1.97	0.47
1:B:411:ARG:HH21	1:B:412:GLN:CG	2.27	0.47
1:A:44:HIS:ND1	1:A:117:ASP:OD2	2.40	0.47
1:B:23:HIS:HD2	4:B:637:HOH:O	1.96	0.47
1:B:33:LYS:HB3	1:B:36:TYR:HE1	1.80	0.47
1:A:451:TRP:HZ3	1:A:457:VAL:HG11	1.79	0.47
1:B:159:LEU:HD22	1:B:380:PHE:HZ	1.80	0.47
1:B:214:ALA:HA	1:B:217:ARG:HD3	1.95	0.47
1:A:3:GLN:O	1:A:7:TYR:HD2	1.98	0.47
1:A:416:ALA:HB2	1:A:426:TYR:CG	2.50	0.47
1:B:166:LYS:HA	1:B:167:PRO:C	2.36	0.47
1:A:122:LYS:HA	1:A:302:GLY:O	2.15	0.46
1:B:15:GLU:CD	1:B:15:GLU:H	2.18	0.46
1:B:191:LYS:HG2	1:B:192:ASN:O	2.15	0.46
1:B:339:ILE:HG22	1:B:343:LEU:HD22	1.96	0.46
1:B:234:ALA:HB3	1:B:240:ILE:HG13	1.98	0.46
1:B:154:GLU:HB3	4:B:510:HOH:O	2.16	0.46
1:A:265:TYR:CD1	1:A:291:HIS:HA	2.50	0.46
1:B:172:ARG:NE	1:B:201:PHE:O	2.49	0.46
1:B:427:ALA:O	1:B:434:ALA:HB2	2.16	0.46
1:A:428:ARG:NE	1:A:454:ALA:O	2.49	0.46
1:B:75:ASP:OD1	1:B:78:ARG:HD3	2.15	0.46
1:A:421:VAL:HA	1:A:422:PRO:HD3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LYS:HD2	1:B:120:TYR:CZ	2.51	0.45
1:A:265:TYR:HB3	1:A:289:ALA:O	2.16	0.45
1:B:168:LYS:NZ	1:B:194:GLU:OE2	2.50	0.45
1:B:322:THR:CG2	1:B:323:GLY:H	2.11	0.45
1:B:372:ASN:HD21	1:B:443:ASP:CG	2.19	0.45
1:A:112:ASN:HA	1:A:115:MET:SD	2.57	0.45
1:A:3:GLN:C	1:A:4:SER:O	2.54	0.45
1:A:4:SER:O	1:A:6:ARG:N	2.46	0.45
1:A:376:MET:CB	1:A:377:PRO:HD3	2.45	0.45
1:A:53:THR:HG22	1:A:54:ASN:N	2.32	0.45
1:B:321:HIS:HE1	1:B:324:THR:HG23	1.81	0.45
1:B:119:GLU:O	1:B:119:GLU:HG2	2.17	0.44
1:A:113:GLN:O	1:B:292:GLY:HA3	2.16	0.44
1:A:337:ARG:NH2	1:A:337:ARG:HB2	2.32	0.44
1:A:281:ASP:HB2	4:A:525:HOH:O	2.18	0.44
1:A:10:LEU:O	1:A:11:ALA:HB2	2.18	0.44
1:A:146:LEU:H	1:A:146:LEU:HD12	1.81	0.44
1:A:404:VAL:HA	4:A:515:HOH:O	2.17	0.44
1:A:238:PHE:HE2	1:B:238:PHE:CZ	2.35	0.44
1:A:450:GLY:O	1:A:452:ARG:N	2.50	0.44
1:B:105:LEU:O	1:B:109:MET:HB3	2.17	0.43
1:B:152:ARG:HA	4:B:704:HOH:O	2.18	0.43
1:B:190:ILE:O	1:B:228:PHE:HA	2.19	0.43
1:B:112:ASN:HA	1:B:115:MET:CG	2.47	0.43
1:A:342:MET:HA	1:A:348:ALA:CB	2.48	0.43
1:B:174:LYS:HB3	1:B:175:PRO:HD3	2.00	0.43
1:B:120:TYR:HB2	1:B:300:LYS:O	2.18	0.43
1:B:165:ILE:CG2	1:B:176:PHE:CE2	2.99	0.43
1:A:205:ARG:HG2	1:A:246:TYR:CZ	2.54	0.43
1:B:431:LYS:HA	1:B:431:LYS:NZ	2.33	0.43
1:A:104:PHE:HE2	1:A:311:MET:CE	2.31	0.43
1:A:89:LEU:HD22	1:B:169:LEU:HD23	2.01	0.43
1:B:376:MET:HG3	1:B:380:PHE:CE2	2.53	0.43
1:B:291:HIS:O	1:B:295:THR:HB	2.19	0.43
1:A:366:ILE:HG12	1:A:389:ILE:HB	2.01	0.42
1:B:425:ASP:CG	1:B:428:ARG:HH11	2.22	0.42
1:A:199:GLN:HA	1:A:200:PRO:HD2	1.81	0.42
1:A:25:LEU:HD23	4:A:626:HOH:O	2.19	0.42
1:A:3:GLN:N	1:A:3:GLN:OE1	2.48	0.42
1:A:181:HIS:HB2	1:A:214:ALA:HB1	2.01	0.42
1:A:445:ASP:HB3	1:A:451:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:THR:O	1:B:325:MET:CB	2.66	0.42
1:B:408:ARG:NH1	4:B:682:HOH:O	2.52	0.42
1:A:243:ARG:O	1:A:247:VAL:HG13	2.20	0.42
1:A:408:ARG:HH21	1:A:408:ARG:HD3	1.69	0.42
1:A:451:TRP:O	1:A:455:LEU:HB2	2.19	0.42
1:A:268:GLY:O	1:A:271:ALA:HB3	2.20	0.42
1:B:337:ARG:HH21	1:B:382:ASN:HD22	1.66	0.42
1:A:167:PRO:HD2	1:A:171:LEU:HD13	2.02	0.42
1:A:167:PRO:HD2	1:A:171:LEU:CD1	2.50	0.42
1:A:266:VAL:HG21	1:B:106:THR:OG1	2.19	0.42
1:B:339:ILE:O	1:B:343:LEU:HB2	2.20	0.42
1:B:447:ILE:C	1:B:449:PRO:HD3	2.39	0.42
1:B:451:TRP:O	1:B:454:ALA:HB3	2.19	0.42
1:A:376:MET:HG3	1:A:380:PHE:CE2	2.55	0.42
1:A:236:ASP:HA	1:A:237:PRO:HD3	1.81	0.41
1:B:364:THR:HA	1:B:365:PRO:HD3	1.78	0.41
1:A:166:LYS:HA	1:A:167:PRO:C	2.41	0.41
1:B:176:PHE:CE1	1:B:211:VAL:HG21	2.56	0.41
1:B:75:ASP:HA	1:B:76:GLU:OE2	2.21	0.41
1:A:296:SER:HA	1:A:297:PRO:HD3	1.86	0.41
1:B:74:VAL:HA	1:B:80:LEU:O	2.20	0.41
1:A:109:MET:CE	1:A:123:MET:HB2	2.51	0.41
1:A:168:LYS:HD2	1:A:195:PRO:HG3	2.03	0.41
1:A:451:TRP:O	1:A:455:LEU:N	2.47	0.41
1:B:344:THR:HA	1:B:362:ALA:HB1	2.00	0.41
1:B:101:ILE:O	1:B:102:ALA:C	2.58	0.41
1:B:172:ARG:HD3	4:B:707:HOH:O	2.19	0.41
1:B:194:GLU:CG	1:B:195:PRO:HD3	2.46	0.41
1:B:33:LYS:HG3	4:B:746:HOH:O	2.19	0.41
1:B:337:ARG:NH2	1:B:382:ASN:HD22	2.19	0.41
1:B:239:GLU:O	1:B:243:ARG:HG3	2.20	0.41
1:B:324:THR:CG2	1:B:368:SER:HB2	2.50	0.41
1:B:265:TYR:CE2	1:B:291:HIS:HA	2.55	0.41
1:B:337:ARG:C	1:B:337:ARG:HD3	2.41	0.41
1:A:445:ASP:OD2	1:A:452:ARG:NH1	2.51	0.41
1:B:33:LYS:HB3	1:B:36:TYR:CE1	2.56	0.41
1:A:130:GLU:HG2	1:A:133:ARG:HH22	1.85	0.41
1:B:143:ILE:HB	1:B:364:THR:HG21	2.03	0.41
1:A:174:LYS:CB	1:A:175:PRO:HD3	2.31	0.41
1:A:253:GLU:HG2	4:A:521:HOH:O	2.21	0.41
1:B:152:ARG:CB	1:B:153:PRO:CD	2.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLY:O	1:B:327:PHE:CB	2.67	0.41
1:B:424:LEU:O	1:B:428:ARG:HG3	2.20	0.41
1:B:45:PHE:CZ	1:B:112:ASN:HB2	2.55	0.41
1:A:155:VAL:O	1:A:156:ASP:HB2	2.21	0.41
1:A:373:ALA:HB1	1:A:413:ALA:HB2	2.02	0.40
1:B:140:SER:HB2	1:B:276:ARG:CZ	2.51	0.40
1:A:29:ILE:HG12	1:A:124:HIS:ND1	2.37	0.40
1:B:236:ASP:HA	1:B:237:PRO:HD3	1.89	0.40
1:A:276:ARG:HB2	4:A:602:HOH:O	2.20	0.40
1:A:364:THR:HA	1:A:365:PRO:HD3	1.84	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:540:HOH:O	4:B:691:HOH:O[2_645]	0.46	1.74
4:A:661:HOH:O	4:A:779:HOH:O[2_656]	1.54	0.66
4:A:681:HOH:O	4:A:685:HOH:O[2_646]	1.80	0.40
4:A:738:HOH:O	4:B:839:HOH:O[1_545]	1.87	0.33
1:B:327:PHE:O	4:B:690:HOH:O[2_645]	1.89	0.31
1:B:408:ARG:NE	4:B:851:HOH:O[2_745]	1.93	0.27
1:B:431:LYS:CD	4:B:521:HOH:O[2_745]	1.96	0.24
4:B:644:HOH:O	4:B:807:HOH:O[2_755]	1.99	0.21
1:B:431:LYS:CE	4:B:837:HOH:O[2_745]	2.11	0.09
4:A:698:HOH:O	4:B:563:HOH:O[1_455]	2.13	0.07
1:B:333:GLU:CG	4:A:803:HOH:O[2_655]	2.15	0.05
1:B:450:GLY:CA	4:B:833:HOH:O[2_645]	2.18	0.02
4:A:631:HOH:O	4:B:569:HOH:O[1_545]	2.18	0.02

## 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	431/490 (88%)	382 (89%)	34 (8%)	15 (4%)	3	2
1	B	438/490 (89%)	387 (88%)	36 (8%)	15 (3%)	3	2
All	All	869/980 (89%)	769 (88%)	70 (8%)	30 (4%)	3	2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	53	THR
1	A	264	GLY
1	A	443	ASP
1	A	451	TRP
1	B	5	SER
1	B	323	GLY
1	B	327	PHE
1	B	333	GLU
1	B	336	ASP
1	A	21	GLY
1	A	33	LYS
1	A	34	ALA
1	A	117	ASP
1	B	110	GLY
1	B	116	GLY
1	B	291	HIS
1	A	289	ALA
1	B	334	SER
1	A	5	SER
1	A	252	GLY
1	A	449	PRO
1	B	114	GLY
1	A	114	GLY
1	B	53	THR
1	B	120	TYR
1	B	325	MET
1	B	252	GLY
1	B	387	ASN
1	A	52	GLY

### 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	330/376 (88%)	284 (86%)	46 (14%)	3	3
1	B	334/376 (89%)	291 (87%)	43 (13%)	4	4
All	All	664/752 (88%)	575 (87%)	89 (13%)	4	4

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

Mol	Chain	Res	Type
1	A	2	ASP
1	A	5	SER
1	A	17	LEU
1	A	45	PHE
1	A	54	ASN
1	A	65	ARG
1	A	68	ASP
1	A	70	LEU
1	A	74	VAL
1	A	80	LEU
1	A	95	THR
1	A	107	LEU
1	A	111	ASN
1	A	112	ASN
1	A	135	LEU
1	A	142	ASN
1	A	144	SER
1	A	165	ILE
1	A	166	LYS
1	A	168	LYS
1	A	169	LEU
1	A	174	LYS
1	A	175	PRO
1	A	178	GLU
1	A	192	ASN
1	A	248	LEU
1	A	253	GLU
1	A	261	LEU
1	A	278	ARG
1	A	284	LEU
1	A	286	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	294	VAL
1	A	300	LYS
1	A	313	ARG
1	A	336	ASP
1	A	354	ARG
1	A	356	SER
1	A	375	ARG
1	A	376	MET
1	A	383	LEU
1	A	390	LEU
1	A	391	THR
1	A	418	ARG
1	A	448	TYR
1	A	451	TRP
1	A	453	LYS
1	B	15	GLU
1	B	54	ASN
1	B	67	VAL
1	B	74	VAL
1	B	109	MET
1	B	111	ASN
1	B	112	ASN
1	B	115	MET
1	B	154	GLU
1	B	156	ASP
1	B	163	THR
1	B	164	ILE
1	B	169	LEU
1	B	172	ARG
1	B	194	GLU
1	B	204	LEU
1	B	206	ASP
1	B	217	ARG
1	B	222	THR
1	B	227	LEU
1	B	229	SER
1	B	249	GLU
1	B	253	GLU
1	B	257	HIS
1	B	261	LEU
1	B	286	TYR
1	B	291	HIS

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Mol	Chain	Res	Type
1	B	295	THR
1	B	304	THR
1	B	324	THR
1	B	327	PHE
1	B	329	LYS
1	B	333	GLU
1	B	336	ASP
1	B	337	ARG
1	B	343	LEU
1	B	354	ARG
1	B	361	LYS
1	B	367	ILE
1	B	411	ARG
1	B	424	LEU
1	B	431	LYS
1	B	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	93	ASN
1	A	112	ASN
1	A	124	HIS
1	A	142	ASN
1	A	219	GLN
1	A	308	HIS
1	A	315	GLN
1	A	349	GLN
1	B	23	HIS
1	B	257	HIS
1	B	287	HIS
1	B	298	GLN
1	B	308	HIS
1	B	315	GLN
1	B	349	GLN
1	B	382	ASN
1	B	387	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	FOR	B	501	1	0,1,1	0.00	-	-		
3	FOR	A	501	1,2	0,1,1	0.00	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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.