



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:31 PM UTC

PDB ID : 2RUS / pdb_00002rus
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)

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A user guide is available at

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

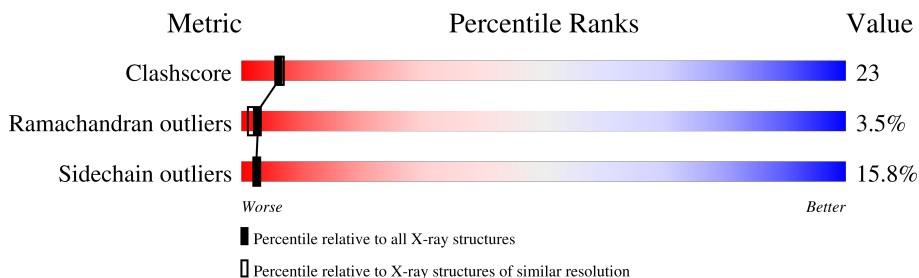
1 Overall quality at a glance

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

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
1	A	437	Total	C	N	O	S	14	0	0
			3339	2115	590	619	15			
1	B	444	Total	C	N	O	S	28	0	0
			3386	2145	598	627	16			

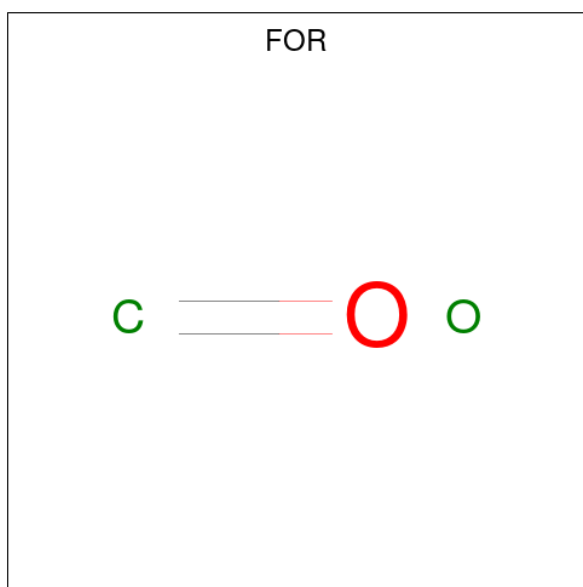
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is FORMYL GROUP (CCD ID: FOR) (formula: CH₂O).



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.

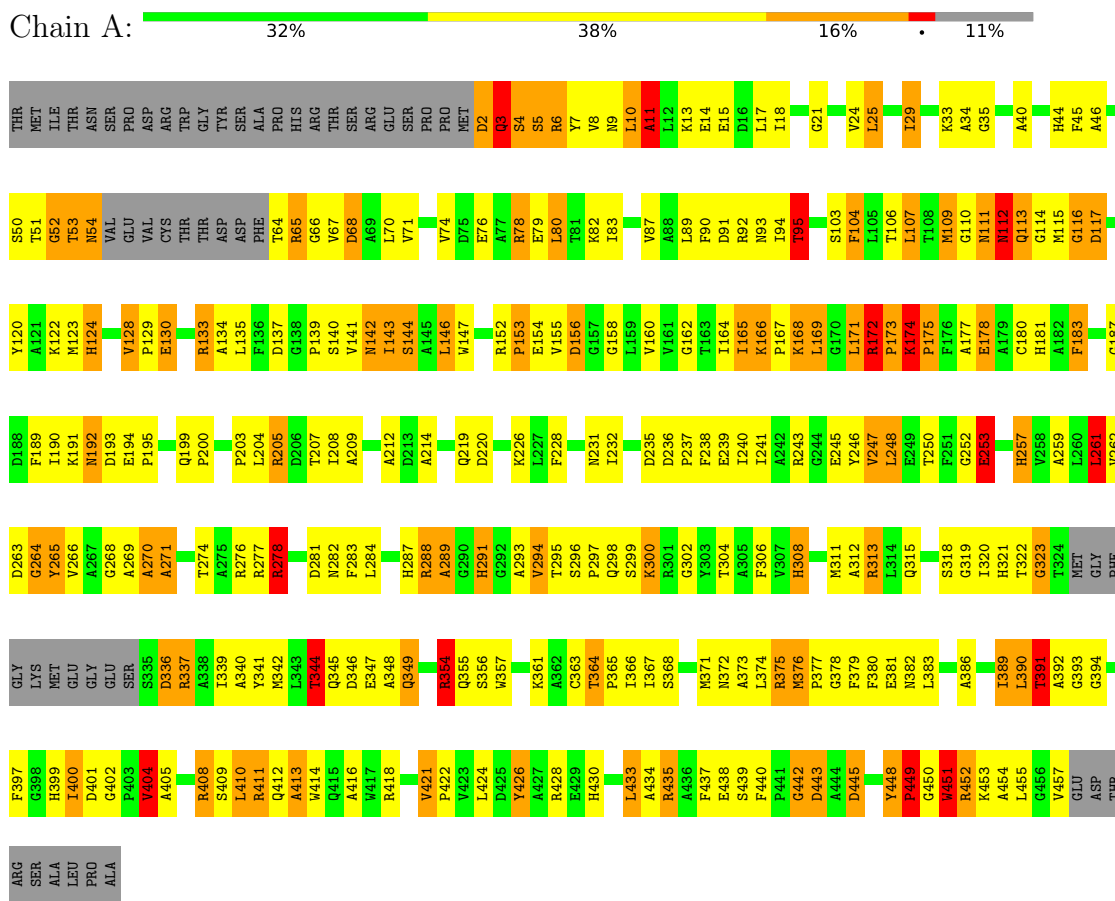
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	340	Total	O	0	0
			340	340		
4	B	374	Total	O	0	0
			374	374		

3 Residue-property plots

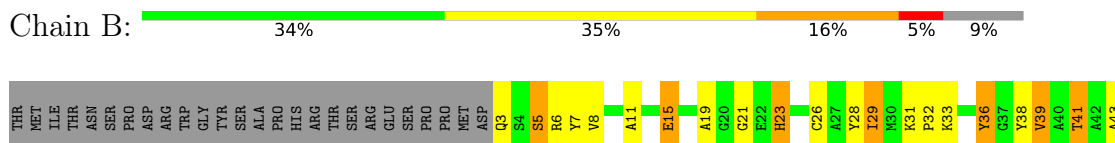
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

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



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



H44	M123	E194	L260	F327	V404	A405	G328	L261	V266	F327	G332	R333	S334	S335	D336	R337	A338	I339	A340	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA
F45	M123	P195	L261	G328	A405	G406	K329	V262	V266	S334	G332	E333	S334	S335	D336	R337	A338	I339	A340	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA
A46	M123	Q196	L262	K329	A406	G407	MET	G263	V267	S335	G333	E334	R411	Q412	A413	W414	Q415	A416	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA	
A47	M124	P196	V262	K329	A407	G408	GLU	G264	V267	S336	G332	E333	R411	Q412	A413	W414	Q415	A416	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA	
E48	D125	G197	G263	D263	S409	R408	GLU	G264	V268	S336	G333	E334	R412	Q413	A414	W415	Q416	A417	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA	
S49	Y127	N198	Y265	Y265	S409	R409	G332	Y265	V268	S336	G333	E334	R412	Q413	A414	W415	Q416	A417	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA	
S50	R133	A201	V266	V266	L410	R411	E333	A201	V267	S334	G332	E333	R412	Q413	A414	W415	Q416	A417	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA	
T51	F136	P201	V267	A267	L411	R412	E334	A202	V267	S334	G332	E333	R412	Q413	A414	W415	Q416	A417	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA	
N54	D137	P203	L204	G268	A269	R337	A270	R205	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
VAL	G138	R205	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
GLU	P139	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
VAL	S140	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
CYS	V141	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
THR	N142	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
THR	I143	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
ASP	L146	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
ASP	W147	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
PHE	K148	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
PHE	R148	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
T64	L150	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
V67	G151	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
D68	G152	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
A69	R152	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
V74	E154	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
D75	G158	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
E76	L159	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
A77	V160	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
R78	V161	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R220	E221	Y222	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259		
E79	G162	R206	L204	G269	A270	R337	A271	R206	D206	T207	I208	A209	L210	V211	A212	D213	A																																						

4 Data and refinement statistics

Xtriage (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, α , β , γ	65.50 Å 70.60 Å 104.10 Å 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.	Xtriage
Total number of atoms	7447	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: 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	1.08	3/3419 (0.1%)	2.56	254/4633 (5.5%)
1	B	1.08	4/3467 (0.1%)	2.58	275/4694 (5.9%)
All	All	1.08	7/6886 (0.1%)	2.57	529/9327 (5.7%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	GLY	C-N	-7.44	1.23	1.33
1	A	165	ILE	N-CA	6.26	1.53	1.46
1	A	295	THR	CA-CB	5.97	1.59	1.53
1	B	3	GLN	C-N	-5.65	1.25	1.33
1	B	165	ILE	CA-CB	5.52	1.60	1.54
1	A	169	LEU	N-CA	5.23	1.52	1.46
1	B	190	ILE	C-N	-5.08	1.26	1.33

All (529) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	CD-NE-CZ	34.89	173.25	124.40
1	B	375	ARG	CD-NE-CZ	21.89	155.04	124.40
1	B	165	ILE	N-CA-CB	-21.16	86.87	111.00
1	A	3	GLN	CA-C-O	14.14	136.96	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ASN	CA-CB-CG	-13.11	99.49	112.60
1	B	445	ASP	CA-CB-CG	13.11	125.71	112.60
1	B	372	ASN	CA-CB-CG	13.11	125.71	112.60
1	B	328	GLY	O-C-N	12.33	138.73	122.70
1	A	68	ASP	CA-CB-CG	12.33	124.93	112.60
1	B	457	VAL	CA-C-O	-12.29	99.90	120.80
1	A	445	ASP	CA-CB-CG	12.19	124.79	112.60
1	A	116	GLY	N-CA-C	-11.61	94.78	111.03
1	A	263	ASP	CA-CB-CG	11.34	123.94	112.60
1	A	10	LEU	CA-C-O	-11.12	107.38	120.62
1	B	337	ARG	CD-NE-CZ	11.09	139.92	124.40
1	B	133	ARG	CD-NE-CZ	10.90	139.66	124.40
1	A	263	ASP	CA-C-N	10.88	142.72	121.41
1	A	263	ASP	C-N-CA	10.88	142.72	121.41
1	A	45	PHE	CA-CB-CG	10.77	124.57	113.80
1	B	172	ARG	CG-CD-NE	10.52	135.15	112.00
1	A	205	ARG	NE-CZ-NH2	10.44	128.60	119.20
1	A	10	LEU	N-CA-C	-10.35	94.25	109.15
1	B	165	ILE	CB-CA-C	10.31	123.44	110.96
1	A	112	ASN	CA-CB-CG	10.30	122.90	112.60
1	B	428	ARG	CD-NE-CZ	10.06	138.48	124.40
1	A	193	ASP	N-CA-C	-10.01	98.10	110.41
1	B	189	PHE	CA-CB-CG	9.82	123.62	113.80
1	A	93	ASN	CA-CB-CG	9.72	122.32	112.60
1	B	192	ASN	CA-CB-CG	9.57	122.17	112.60
1	A	91	ASP	CA-CB-CG	9.54	122.14	112.60
1	B	75	ASP	CA-C-O	9.29	130.39	120.63
1	A	318	SER	CA-C-N	9.21	132.61	121.38
1	A	318	SER	C-N-CA	9.21	132.61	121.38
1	B	75	ASP	CA-C-N	9.19	132.95	120.54
1	B	75	ASP	C-N-CA	9.19	132.95	120.54
1	A	203	PRO	CA-C-N	9.08	132.79	120.54
1	A	203	PRO	C-N-CA	9.08	132.79	120.54
1	A	111	ASN	CA-CB-CG	9.03	121.63	112.60
1	A	313	ARG	NE-CZ-NH2	9.00	127.30	119.20
1	B	201	PHE	CA-CB-CG	8.96	122.76	113.80
1	B	5	SER	CA-C-N	8.83	137.90	122.09
1	B	5	SER	C-N-CA	8.83	137.90	122.09
1	B	68	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	393	GLY	N-CA-C	-8.76	101.33	112.54
1	A	291	HIS	CA-C-N	8.66	138.38	121.41
1	A	291	HIS	C-N-CA	8.66	138.38	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASN	CA-CB-CG	8.59	121.19	112.60
1	B	109	MET	N-CA-CB	-8.56	96.03	110.49
1	B	327	PHE	CA-CB-CG	8.53	122.33	113.80
1	B	335	SER	N-CA-C	8.49	122.89	110.59
1	A	291	HIS	CA-CB-CG	-8.47	105.33	113.80
1	B	112	ASN	CA-CB-CG	8.47	121.07	112.60
1	B	283	PHE	CA-CB-CG	8.47	122.27	113.80
1	A	430	HIS	CA-CB-CG	-8.47	105.33	113.80
1	B	414	TRP	CA-C-N	8.42	131.39	120.44
1	B	414	TRP	C-N-CA	8.42	131.39	120.44
1	B	282	ASN	OD1-CG-ND2	8.40	131.00	122.60
1	B	238	PHE	CA-CB-CG	-8.38	105.42	113.80
1	B	212	ALA	CA-C-N	8.37	131.82	120.44
1	B	212	ALA	C-N-CA	8.37	131.82	120.44
1	A	94	ILE	CA-C-O	8.29	129.20	120.25
1	B	271	ALA	N-CA-C	-8.26	101.97	110.97
1	B	338	ALA	CA-C-N	8.24	131.75	120.46
1	B	338	ALA	C-N-CA	8.24	131.75	120.46
1	A	245	GLU	CA-CB-CG	8.21	130.52	114.10
1	A	116	GLY	CA-C-O	-8.21	113.26	120.98
1	A	165	ILE	N-CA-CB	-8.20	101.59	110.53
1	A	165	ILE	O-C-N	8.14	131.84	122.81
1	B	382	ASN	OD1-CG-ND2	8.11	130.71	122.60
1	A	274	THR	CA-C-N	8.11	130.98	120.44
1	A	274	THR	C-N-CA	8.11	130.98	120.44
1	B	308	HIS	CA-C-N	8.10	130.96	120.44
1	B	308	HIS	C-N-CA	8.10	130.96	120.44
1	B	367	ILE	CB-CA-C	8.08	122.69	111.38
1	A	271	ALA	CA-C-N	8.07	131.51	120.46
1	A	271	ALA	C-N-CA	8.07	131.51	120.46
1	A	386	ALA	CA-C-N	8.05	136.92	121.54
1	A	386	ALA	C-N-CA	8.05	136.92	121.54
1	B	304	THR	N-CA-CB	-8.05	98.85	110.36
1	A	95	THR	CA-CB-CG2	8.03	124.16	110.50
1	B	421	VAL	O-C-N	8.02	128.63	121.41
1	B	6	ARG	N-CA-C	-7.99	103.66	113.41
1	B	193	ASP	N-CA-C	-7.96	98.70	110.48
1	B	269	ALA	CA-C-O	-7.96	112.03	120.63
1	A	3	GLN	N-CA-CB	7.88	121.97	109.51
1	A	177	ALA	CA-C-N	7.83	130.62	120.44
1	A	177	ALA	C-N-CA	7.83	130.62	120.44
1	A	282	ASN	CA-CB-CG	-7.82	104.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NE-CZ-NH1	-7.79	113.71	121.50
1	B	124	HIS	CA-CB-CG	-7.79	106.02	113.80
1	B	267	ALA	N-CA-C	-7.78	104.27	114.31
1	B	3	GLN	CA-C-N	7.73	136.31	121.54
1	B	3	GLN	C-N-CA	7.73	136.31	121.54
1	A	45	PHE	N-CA-C	-7.73	102.94	111.36
1	B	436	ALA	N-CA-C	-7.72	102.20	111.69
1	B	290	GLY	CA-C-N	7.71	136.27	121.54
1	B	290	GLY	C-N-CA	7.71	136.27	121.54
1	A	349	GLN	CA-C-O	-7.68	112.09	120.30
1	A	205	ARG	CD-NE-CZ	7.67	135.14	124.40
1	A	4	SER	N-CA-C	-7.66	94.47	110.80
1	A	404	VAL	N-CA-C	-7.64	103.40	110.82
1	A	46	ALA	CA-C-N	7.62	130.34	120.44
1	A	46	ALA	C-N-CA	7.62	130.34	120.44
1	A	253	GLU	CB-CG-CD	7.62	125.55	112.60
1	B	275	ALA	CA-C-O	-7.60	112.84	120.82
1	B	67	VAL	N-CA-CB	-7.60	102.06	111.94
1	A	192	ASN	N-CA-C	-7.58	99.26	110.48
1	A	364	THR	N-CA-C	7.53	120.57	109.50
1	A	129	PRO	CA-C-N	7.51	130.21	120.44
1	A	129	PRO	C-N-CA	7.51	130.21	120.44
1	A	391	THR	CB-CA-C	7.50	122.78	111.76
1	B	175	PRO	CA-C-N	7.47	130.15	120.44
1	B	175	PRO	C-N-CA	7.47	130.15	120.44
1	B	294	VAL	N-CA-C	7.44	118.21	111.81
1	B	266	VAL	N-CA-C	7.39	122.60	113.00
1	B	203	PRO	CA-C-N	7.38	131.04	120.79
1	B	203	PRO	C-N-CA	7.38	131.04	120.79
1	B	389	ILE	N-CA-CB	7.37	121.28	111.25
1	A	94	ILE	CA-C-N	7.36	135.61	121.54
1	A	94	ILE	C-N-CA	7.36	135.61	121.54
1	B	412	GLN	CA-C-N	7.34	130.12	120.28
1	B	412	GLN	C-N-CA	7.34	130.12	120.28
1	B	363	CYS	CB-CA-C	7.32	123.11	109.71
1	A	134	ALA	CA-C-N	7.30	133.09	120.68
1	A	134	ALA	C-N-CA	7.30	133.09	120.68
1	B	243	ARG	CA-C-N	7.29	128.22	119.99
1	B	243	ARG	C-N-CA	7.29	128.22	119.99
1	A	141	VAL	CA-C-O	-7.28	114.50	121.64
1	B	294	VAL	CA-C-N	7.27	130.61	120.29
1	B	294	VAL	C-N-CA	7.27	130.61	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	THR	N-CA-CB	-7.25	99.41	110.13
1	A	277	ARG	NE-CZ-NH1	7.22	128.72	121.50
1	A	207	THR	CA-C-O	-7.20	113.20	120.90
1	A	25	LEU	CB-CA-C	7.19	123.10	109.37
1	B	11	ALA	N-CA-C	-7.18	104.55	113.38
1	A	6	ARG	NE-CZ-NH1	-7.18	114.32	121.50
1	A	147	TRP	CA-C-O	-7.14	113.26	120.90
1	A	141	VAL	O-C-N	7.11	130.84	122.95
1	B	76	GLU	CB-CG-CD	7.11	124.68	112.60
1	A	344	THR	N-CA-C	7.09	120.05	111.40
1	A	240	ILE	CA-C-N	7.08	130.16	120.46
1	A	240	ILE	C-N-CA	7.08	130.16	120.46
1	B	222	THR	N-CA-CB	-7.08	101.48	110.90
1	A	257	HIS	O-C-N	7.08	131.19	122.34
1	A	66	GLY	CA-C-N	7.06	132.62	122.09
1	A	66	GLY	C-N-CA	7.06	132.62	122.09
1	B	416	ALA	CA-C-N	7.06	129.62	120.44
1	B	416	ALA	C-N-CA	7.06	129.62	120.44
1	B	176	PHE	CA-C-N	7.06	129.73	120.28
1	B	176	PHE	C-N-CA	7.06	129.73	120.28
1	B	127	TYR	CA-C-O	-7.04	112.78	120.24
1	B	328	GLY	CA-C-O	-7.01	108.37	120.57
1	A	90	PHE	CB-CA-C	6.99	121.60	109.65
1	A	435	ARG	NE-CZ-NH1	6.98	128.48	121.50
1	A	109	MET	N-CA-CB	-6.97	98.71	110.49
1	A	130	GLU	N-CA-C	6.95	118.50	111.07
1	A	247	VAL	CA-C-N	6.95	129.59	120.28
1	A	247	VAL	C-N-CA	6.95	129.59	120.28
1	B	263	ASP	CA-C-N	6.94	129.03	120.22
1	B	263	ASP	C-N-CA	6.94	129.03	120.22
1	A	336	ASP	N-CA-C	-6.92	104.98	113.50
1	B	164	ILE	N-CA-CB	6.90	123.39	111.39
1	A	189	PHE	CA-CB-CG	6.89	120.69	113.80
1	B	198	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	345	GLN	N-CA-C	6.82	119.76	110.55
1	B	67	VAL	CB-CA-C	6.82	121.70	112.36
1	A	339	ILE	N-CA-C	-6.81	103.70	110.30
1	A	287	HIS	CA-CB-CG	-6.79	107.01	113.80
1	B	80	LEU	CA-C-N	6.79	132.57	122.99
1	B	80	LEU	C-N-CA	6.79	132.57	122.99
1	B	422	PRO	CA-C-N	6.76	129.72	120.46
1	B	422	PRO	C-N-CA	6.76	129.72	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	GLY	CA-C-N	6.76	130.35	120.82
1	A	158	GLY	C-N-CA	6.76	130.35	120.82
1	A	142	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	B	29	ILE	N-CA-C	-6.74	97.28	106.85
1	B	430	HIS	CA-CB-CG	-6.74	107.06	113.80
1	B	102	ALA	CA-C-O	-6.74	113.37	120.92
1	A	92	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	A	354	ARG	CD-NE-CZ	6.73	133.82	124.40
1	A	313	ARG	CG-CD-NE	6.72	126.78	112.00
1	B	154	GLU	CA-CB-CG	6.71	127.52	114.10
1	B	172	ARG	CB-CA-C	6.68	121.55	109.45
1	B	213	ASP	CA-CB-CG	-6.67	105.93	112.60
1	B	140	SER	CA-C-N	6.66	131.23	122.51
1	B	140	SER	C-N-CA	6.66	131.23	122.51
1	A	3	GLN	CA-C-N	6.64	134.22	121.54
1	A	3	GLN	C-N-CA	6.64	134.22	121.54
1	B	354	ARG	N-CA-C	-6.63	98.82	109.96
1	B	236	ASP	CA-C-N	6.62	126.86	119.32
1	B	236	ASP	C-N-CA	6.62	126.86	119.32
1	B	115	MET	N-CA-C	6.61	124.89	110.80
1	A	337	ARG	CA-C-O	-6.61	112.90	120.24
1	B	108	THR	N-CA-C	6.61	120.60	112.54
1	B	216	ARG	CD-NE-CZ	-6.60	115.16	124.40
1	B	80	LEU	CA-C-O	6.60	127.58	120.32
1	B	74	VAL	CB-CA-C	6.59	123.05	111.18
1	A	264	GLY	N-CA-C	6.59	128.80	113.18
1	B	143	ILE	CA-C-N	6.57	129.74	120.28
1	B	143	ILE	C-N-CA	6.57	129.74	120.28
1	A	270	ALA	CA-C-N	6.56	128.96	120.44
1	A	270	ALA	C-N-CA	6.56	128.96	120.44
1	B	281	ASP	CA-CB-CG	-6.55	106.05	112.60
1	B	335	SER	CA-C-O	6.54	129.55	121.89
1	A	414	TRP	N-CA-C	-6.54	104.08	111.14
1	B	44	HIS	CA-C-N	6.54	129.34	120.38
1	B	44	HIS	C-N-CA	6.54	129.34	120.38
1	B	411	ARG	N-CA-C	-6.54	104.08	111.07
1	B	388	VAL	N-CA-CB	-6.52	102.63	112.35
1	B	297	PRO	CA-C-N	6.49	129.31	120.54
1	B	297	PRO	C-N-CA	6.49	129.31	120.54
1	A	183	PHE	N-CA-CB	6.49	119.76	110.16
1	A	386	ALA	N-CA-CB	-6.49	102.13	111.54
1	A	133	ARG	NE-CZ-NH1	-6.47	115.03	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	TRP	O-C-N	6.47	128.82	122.09
1	A	71	VAL	N-CA-C	-6.44	98.38	108.23
1	B	397	PHE	CA-C-O	-6.44	113.68	120.63
1	A	452	ARG	CD-NE-CZ	6.43	133.41	124.40
1	B	239	GLU	N-CA-C	-6.42	103.79	111.69
1	A	189	PHE	N-CA-CB	-6.41	99.67	110.83
1	A	269	ALA	N-CA-C	6.41	119.25	111.82
1	B	364	THR	N-CA-C	6.38	117.70	109.72
1	A	35	GLY	CA-C-O	6.37	125.74	119.37
1	B	221	GLU	N-CA-C	6.36	120.64	113.01
1	B	305	ALA	N-CA-C	-6.36	103.87	111.69
1	A	24	VAL	N-CA-C	-6.35	99.21	108.87
1	B	182	ALA	CA-C-O	-6.35	114.10	120.90
1	B	249	GLU	CA-C-N	6.34	128.78	120.28
1	B	249	GLU	C-N-CA	6.34	128.78	120.28
1	A	394	GLY	CA-C-N	6.33	128.31	120.34
1	A	394	GLY	C-N-CA	6.33	128.31	120.34
1	B	80	LEU	CB-CA-C	6.33	120.57	110.19
1	B	184	TRP	CA-CB-CG	6.32	125.61	113.60
1	B	225	ALA	CA-C-O	6.29	127.65	120.54
1	B	68	ASP	O-C-N	6.29	130.43	123.01
1	B	159	LEU	N-CA-C	6.29	119.39	109.96
1	B	45	PHE	CA-CB-CG	6.24	120.04	113.80
1	B	183	PHE	CA-C-N	6.24	129.26	120.28
1	B	183	PHE	C-N-CA	6.24	129.26	120.28
1	A	308	HIS	CA-C-N	6.23	129.14	120.29
1	A	308	HIS	C-N-CA	6.23	129.14	120.29
1	B	158	GLY	N-CA-C	6.23	123.84	112.37
1	A	146	LEU	CA-C-O	-6.22	114.29	120.70
1	B	354	ARG	CD-NE-CZ	6.22	133.11	124.40
1	A	355	GLN	OE1-CD-NE2	6.22	128.82	122.60
1	B	180	CYS	CA-C-N	6.20	129.41	120.79
1	B	180	CYS	C-N-CA	6.20	129.41	120.79
1	B	194	GLU	CA-CB-CG	6.20	126.49	114.10
1	A	180	CYS	O-C-N	6.19	129.20	122.15
1	A	259	ALA	N-CA-C	-6.18	100.21	110.17
1	B	110	GLY	CA-C-N	6.18	129.40	120.38
1	B	110	GLY	C-N-CA	6.18	129.40	120.38
1	A	2	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	341	TYR	CA-C-N	6.17	128.55	120.28
1	A	341	TYR	C-N-CA	6.17	128.55	120.28
1	A	263	ASP	N-CA-CB	6.17	119.96	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	ARG	CA-C-O	6.17	127.48	121.00
1	B	41	THR	CA-C-N	6.15	128.81	120.44
1	B	41	THR	C-N-CA	6.15	128.81	120.44
1	B	260	LEU	O-C-N	6.15	130.23	123.22
1	B	352	PHE	CA-CB-CG	-6.15	107.65	113.80
1	B	336	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	140	SER	N-CA-CB	6.14	119.44	110.47
1	A	146	LEU	N-CA-C	-6.14	104.51	111.14
1	B	83	ILE	CA-C-N	6.12	132.21	123.14
1	B	83	ILE	C-N-CA	6.12	132.21	123.14
1	B	311	MET	CA-C-N	6.11	128.47	120.28
1	B	311	MET	C-N-CA	6.11	128.47	120.28
1	A	313	ARG	NH1-CZ-NH2	-6.11	111.36	119.30
1	A	405	ALA	O-C-N	6.09	128.58	122.12
1	B	126	PHE	CA-CB-CG	6.09	119.89	113.80
1	B	229	SER	CA-C-O	-6.09	113.76	120.70
1	B	337	ARG	CB-CG-CD	6.09	125.31	111.30
1	B	164	ILE	CA-C-O	6.09	127.80	120.67
1	A	68	ASP	CA-C-N	6.08	131.05	121.99
1	A	68	ASP	C-N-CA	6.08	131.05	121.99
1	B	160	VAL	CA-C-O	-6.08	114.03	120.53
1	A	51	THR	CA-CB-OG1	-6.08	100.49	109.60
1	A	67	VAL	N-CA-CB	-6.08	101.87	112.08
1	A	354	ARG	N-CA-CB	6.04	120.49	110.52
1	B	23	HIS	CA-C-O	-6.03	114.05	121.11
1	B	388	VAL	O-C-N	6.03	129.64	122.95
1	B	197	GLY	O-C-N	6.02	130.53	122.70
1	B	36	TYR	CA-CB-CG	6.01	124.72	113.90
1	B	79	GLU	O-C-N	6.01	129.79	122.58
1	A	288	ARG	N-CA-C	6.00	120.29	113.15
1	B	353	TYR	N-CA-C	5.99	119.25	109.24
1	A	278	ARG	CD-NE-CZ	5.99	132.79	124.40
1	B	207	THR	CA-CB-OG1	-5.98	100.64	109.60
1	B	211	VAL	CA-C-N	5.97	128.28	120.28
1	B	211	VAL	C-N-CA	5.97	128.28	120.28
1	A	143	ILE	CA-C-O	-5.96	112.81	120.03
1	B	146	LEU	O-C-N	5.96	128.53	122.09
1	A	364	THR	CA-CB-OG1	-5.96	100.67	109.60
1	B	205	ARG	CD-NE-CZ	-5.95	116.06	124.40
1	A	247	VAL	CB-CA-C	5.95	119.59	111.97
1	A	209	ALA	N-CA-C	-5.94	104.71	111.07
1	B	346	ASP	CA-C-O	5.94	125.67	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	ARG	CD-NE-CZ	-5.94	116.08	124.40
1	A	357	TRP	O-C-N	5.93	129.42	122.24
1	A	361	LYS	CA-C-O	5.92	128.98	120.51
1	A	139	PRO	CA-C-O	-5.91	114.60	121.34
1	B	152	ARG	CA-CB-CG	-5.89	102.31	114.10
1	A	130	GLU	CA-C-N	5.89	128.17	120.28
1	A	130	GLU	C-N-CA	5.89	128.17	120.28
1	B	408	ARG	NE-CZ-NH2	-5.88	113.91	119.20
1	A	160	VAL	CA-C-O	-5.88	114.24	120.53
1	B	218	ALA	CA-C-O	-5.87	114.29	120.63
1	B	53	THR	O-C-N	5.86	130.39	122.59
1	B	50	SER	CA-C-N	5.86	128.41	120.44
1	B	50	SER	C-N-CA	5.86	128.41	120.44
1	A	354	ARG	N-CA-C	-5.85	100.16	109.76
1	A	144	SER	N-CA-CB	5.85	119.23	110.22
1	A	110	GLY	CA-C-N	5.84	128.91	120.38
1	A	110	GLY	C-N-CA	5.84	128.91	120.38
1	B	369	GLY	N-CA-C	5.84	122.89	112.02
1	B	45	PHE	CA-C-O	-5.84	114.32	120.63
1	B	337	ARG	N-CA-CB	5.81	120.55	110.44
1	A	190	ILE	O-C-N	5.81	129.32	123.10
1	A	71	VAL	CA-C-O	-5.81	113.86	120.65
1	B	322	THR	CA-C-O	5.80	129.18	121.47
1	B	46	ALA	CA-C-N	5.80	128.30	120.65
1	B	46	ALA	C-N-CA	5.80	128.30	120.65
1	B	253	GLU	CB-CG-CD	5.79	122.45	112.60
1	A	154	GLU	O-C-N	5.79	130.19	122.43
1	A	382	ASN	CA-CB-CG	-5.78	106.82	112.60
1	A	144	SER	CB-CA-C	-5.76	99.98	110.63
1	B	201	PHE	CA-C-N	5.76	129.18	122.85
1	B	201	PHE	C-N-CA	5.76	129.18	122.85
1	B	259	ALA	N-CA-C	-5.75	100.80	109.95
1	B	209	ALA	CA-C-O	-5.75	114.77	120.70
1	A	189	PHE	N-CA-C	5.74	118.75	109.40
1	B	277	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	A	146	LEU	CB-CA-C	5.73	119.96	110.90
1	B	391	THR	CA-C-N	5.73	129.00	120.87
1	B	391	THR	C-N-CA	5.73	129.00	120.87
1	B	188	ASP	N-CA-C	5.71	120.26	113.12
1	A	109	MET	CA-CB-CG	5.71	125.51	114.10
1	B	19	ALA	CA-C-N	5.70	127.46	120.22
1	B	19	ALA	C-N-CA	5.70	127.46	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	262	VAL	O-C-N	5.67	129.33	123.20
1	A	239	GLU	N-CA-C	-5.66	104.73	111.69
1	B	109	MET	CA-C-N	5.65	132.49	121.41
1	B	109	MET	C-N-CA	5.65	132.49	121.41
1	A	79	GLU	CB-CG-CD	5.64	122.19	112.60
1	A	154	GLU	CA-C-O	-5.64	112.44	119.38
1	A	78	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	B	316	GLY	O-C-N	5.63	130.02	122.70
1	A	409	SER	CA-C-N	5.62	128.09	120.44
1	A	409	SER	C-N-CA	5.62	128.09	120.44
1	A	408	ARG	CA-C-N	5.61	127.79	120.28
1	A	408	ARG	C-N-CA	5.61	127.79	120.28
1	B	164	ILE	N-CA-C	-5.61	100.41	108.48
1	B	265	TYR	CB-CA-C	5.59	119.61	110.95
1	B	340	ALA	CA-C-N	5.59	128.22	120.29
1	B	340	ALA	C-N-CA	5.59	128.22	120.29
1	B	271	ALA	O-C-N	5.57	127.82	122.03
1	A	208	ILE	N-CA-C	5.57	116.30	110.62
1	A	173	PRO	CA-C-N	5.56	127.67	120.44
1	A	173	PRO	C-N-CA	5.56	127.67	120.44
1	B	294	VAL	CA-C-O	5.53	126.41	120.32
1	A	411	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	B	235	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	268	GLY	CA-C-N	5.53	127.95	120.38
1	B	268	GLY	C-N-CA	5.53	127.95	120.38
1	B	383	LEU	CB-CA-C	5.53	120.25	110.85
1	B	120	TYR	CA-C-O	5.51	128.40	120.51
1	B	407	ALA	O-C-N	5.51	127.75	122.07
1	B	274	THR	N-CA-C	-5.51	104.91	111.03
1	B	445	ASP	CA-C-O	5.51	126.37	120.70
1	A	78	ARG	CD-NE-CZ	5.50	132.11	124.40
1	B	101	ILE	CA-CB-CG2	5.50	119.86	110.50
1	A	410	LEU	CA-C-O	-5.50	115.03	120.70
1	A	147	TRP	N-CA-CB	5.50	118.13	109.94
1	B	347	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	76	GLU	CB-CG-CD	5.50	121.94	112.60
1	B	316	GLY	CA-C-O	-5.50	111.01	120.57
1	B	105	LEU	CA-C-O	-5.49	115.04	120.70
1	A	346	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	192	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	B	293	ALA	CA-C-N	5.48	128.81	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ALA	C-N-CA	5.48	128.81	122.35
1	A	232	ILE	N-CA-C	-5.47	107.40	112.43
1	B	274	THR	CA-C-O	-5.47	115.27	120.90
1	A	319	GLY	CA-C-O	5.46	126.16	121.19
1	A	413	ALA	O-C-N	-5.46	115.93	122.15
1	B	240	ILE	CA-C-N	5.45	127.63	120.60
1	B	240	ILE	C-N-CA	5.45	127.63	120.60
1	B	368	SER	CB-CA-C	-5.45	100.22	111.22
1	A	378	GLY	CA-C-N	5.44	127.51	120.44
1	A	378	GLY	C-N-CA	5.44	127.51	120.44
1	A	440	PHE	O-C-N	5.44	125.79	121.17
1	B	118	VAL	O-C-N	5.44	128.84	123.18
1	A	313	ARG	CA-CB-CG	5.43	124.97	114.10
1	A	104	PHE	O-C-N	-5.43	116.47	122.07
1	A	378	GLY	N-CA-C	-5.43	106.20	112.50
1	A	137	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	83	ILE	CB-CG1-CD1	5.42	125.19	113.80
1	A	344	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	321	HIS	N-CA-C	-5.39	102.07	110.10
1	B	386	ALA	CA-C-O	-5.38	113.13	119.48
1	B	51	THR	N-CA-C	5.38	116.95	111.14
1	A	147	TRP	N-CA-C	-5.38	104.65	111.11
1	A	401	ASP	N-CA-C	-5.38	106.76	113.38
1	B	411	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	265	TYR	N-CA-C	-5.38	104.30	111.24
1	A	298	GLN	N-CA-C	-5.37	106.00	112.54
1	B	190	ILE	O-C-N	5.36	128.84	123.10
1	B	204	LEU	CA-CB-CG	5.35	135.02	116.30
1	B	28	TYR	CB-CA-C	-5.35	99.29	109.66
1	B	192	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	B	78	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	A	193	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	321	HIS	O-C-N	-5.32	116.32	122.87
1	A	389	ILE	CA-C-O	-5.32	114.84	120.48
1	B	344	THR	N-CA-C	5.32	121.17	114.31
1	A	354	ARG	CA-CB-CG	5.31	124.73	114.10
1	B	372	ASN	N-CA-C	-5.31	102.66	110.52
1	A	92	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	391	THR	CA-CB-CG2	5.29	119.50	110.50
1	B	230	ALA	O-C-N	5.29	129.25	123.27
1	A	220	ASP	CA-CB-CG	-5.29	107.31	112.60
1	B	377	PRO	CA-C-N	5.29	125.82	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	PRO	C-N-CA	5.29	125.82	120.00
1	B	379	PHE	CA-C-N	5.29	127.37	120.28
1	B	379	PHE	C-N-CA	5.29	127.37	120.28
1	B	174	LYS	CA-CB-CG	5.28	124.67	114.10
1	A	128	VAL	O-C-N	5.28	126.44	121.11
1	A	304	THR	CA-CB-CG2	5.28	119.47	110.50
1	B	119	GLU	CA-C-N	5.27	131.61	121.54
1	B	119	GLU	C-N-CA	5.27	131.61	121.54
1	A	40	ALA	CA-C-N	5.27	128.32	120.31
1	A	40	ALA	C-N-CA	5.27	128.32	120.31
1	A	124	HIS	CA-CB-CG	-5.27	108.53	113.80
1	B	245	GLU	CB-CG-CD	5.26	121.55	112.60
1	B	247	VAL	CA-C-O	-5.26	115.59	121.17
1	B	137	ASP	CA-C-O	-5.26	115.48	121.00
1	A	24	VAL	CB-CA-C	5.26	118.41	111.21
1	B	29	ILE	CB-CA-C	5.26	118.36	111.53
1	A	153	PRO	N-CA-CB	5.25	108.23	103.34
1	B	369	GLY	CA-C-O	5.25	128.26	122.01
1	B	67	VAL	CA-CB-CG1	5.25	119.32	110.40
1	A	228	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	442	GLY	N-CA-C	-5.24	100.76	113.18
1	B	415	GLN	N-CA-C	-5.24	105.47	111.07
1	B	176	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	421	VAL	O-C-N	5.23	127.06	121.10
1	B	136	PHE	CA-CB-CG	-5.23	108.57	113.80
1	B	39	VAL	CB-CA-C	5.23	119.19	112.14
1	A	212	ALA	CA-C-N	5.22	128.25	120.31
1	A	212	ALA	C-N-CA	5.22	128.25	120.31
1	B	161	VAL	N-CA-CB	5.22	118.04	111.46
1	A	400	ILE	N-CA-C	5.21	120.18	109.34
1	B	139	PRO	CB-CA-C	5.20	117.89	111.23
1	B	74	VAL	N-CA-CB	-5.20	101.75	111.62
1	B	106	THR	CA-CB-OG1	-5.20	101.81	109.60
1	B	149	VAL	CA-C-O	-5.19	115.87	121.27
1	A	183	PHE	N-CA-C	-5.19	105.70	111.36
1	A	315	GLN	N-CA-CB	5.18	118.32	110.28
1	B	253	GLU	CA-CB-CG	5.18	124.46	114.10
1	B	431	LYS	CA-C-O	-5.17	115.12	120.92
1	B	193	ASP	N-CA-CB	5.17	118.14	110.29
1	B	277	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	B	209	ALA	O-C-N	5.16	127.66	122.09
1	B	314	LEU	N-CA-CB	-5.16	102.33	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	GLY	CA-C-N	5.15	128.16	120.95
1	B	158	GLY	C-N-CA	5.15	128.16	120.95
1	A	315	GLN	O-C-N	5.15	128.61	122.27
1	B	405	ALA	N-CA-C	-5.15	105.74	112.23
1	A	160	VAL	O-C-N	5.15	129.12	123.10
1	A	139	PRO	CB-CA-C	5.15	118.10	111.46
1	B	179	ALA	N-CA-C	-5.15	105.75	111.36
1	B	213	ASP	OD1-CG-OD2	5.15	135.25	122.90
1	A	312	ALA	CA-C-N	5.14	127.44	120.65
1	A	312	ALA	C-N-CA	5.14	127.44	120.65
1	B	54	ASN	CA-CB-CG	-5.14	107.46	112.60
1	A	381	GLU	CA-C-N	5.13	127.11	120.44
1	A	381	GLU	C-N-CA	5.13	127.11	120.44
1	A	411	ARG	N-CA-CB	5.13	117.45	110.01
1	A	405	ALA	N-CA-C	-5.13	105.69	111.28
1	A	368	SER	N-CA-C	5.13	117.33	109.95
1	B	184	TRP	CB-CA-C	5.12	120.11	110.63
1	A	193	ASP	N-CA-CB	5.12	117.39	110.38
1	A	433	LEU	CA-C-O	-5.12	115.43	120.70
1	B	183	PHE	N-CA-CB	5.11	117.63	110.12
1	A	156	ASP	CA-C-N	5.11	129.52	120.74
1	A	156	ASP	C-N-CA	5.11	129.52	120.74
1	A	29	ILE	N-CA-C	-5.11	99.60	106.85
1	A	337	ARG	N-CA-C	5.10	117.97	111.69
1	B	392	ALA	O-C-N	5.10	129.11	122.89
1	A	14	GLU	CB-CG-CD	5.09	121.26	112.60
1	A	248	LEU	CA-C-N	5.09	127.52	120.29
1	A	248	LEU	C-N-CA	5.09	127.52	120.29
1	A	250	THR	CA-CB-OG1	-5.08	101.99	109.60
1	B	305	ALA	CB-CA-C	5.07	119.98	110.70
1	B	69	ALA	CB-CA-C	5.07	118.09	109.53
1	A	323	GLY	CA-C-N	5.06	130.81	121.70
1	A	323	GLY	C-N-CA	5.06	130.81	121.70
1	A	379	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	315	GLN	CA-C-N	-5.06	115.65	122.63
1	A	315	GLN	C-N-CA	-5.06	115.65	122.63
1	A	180	CYS	CA-C-O	-5.05	115.07	120.42
1	B	219	GLN	CA-C-N	5.05	127.30	120.44
1	B	219	GLN	C-N-CA	5.05	127.30	120.44
1	B	313	ARG	O-C-N	-5.05	116.78	122.03
1	A	172	ARG	CA-C-N	5.04	124.22	118.97
1	A	172	ARG	C-N-CA	5.04	124.22	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	TYR	N-CA-C	-5.04	105.48	111.69
1	A	363	CYS	N-CA-C	-5.04	99.04	108.02
1	B	366	ILE	N-CA-C	-5.04	99.26	107.28
1	B	209	ALA	N-CA-C	-5.04	105.70	111.14
1	A	162	GLY	N-CA-C	5.04	118.57	111.42
1	A	172	ARG	CD-NE-CZ	-5.04	117.35	124.40
1	A	346	ASP	CA-C-N	5.03	129.73	121.58
1	A	346	ASP	C-N-CA	5.03	129.73	121.58
1	A	90	PHE	CA-C-O	-5.03	115.52	121.16
1	B	363	CYS	N-CA-C	-5.03	100.70	108.90
1	B	222	THR	CA-CB-CG2	5.03	119.05	110.50
1	A	11	ALA	N-CA-CB	5.03	118.99	110.49
1	A	174	LYS	N-CA-C	-5.02	105.77	112.55
1	B	231	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	9	ASN	CB-CA-C	5.02	120.24	111.86
1	A	261	LEU	N-CA-CB	-5.01	101.89	110.16
1	B	333	GLU	CA-C-N	5.01	131.11	121.54
1	B	333	GLU	C-N-CA	5.01	131.11	121.54
1	A	304	THR	CA-CB-OG1	-5.01	102.09	109.60
1	A	440	PHE	CA-C-N	5.00	124.61	119.05
1	A	440	PHE	C-N-CA	5.00	124.61	119.05

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

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	3239	149	0
1	B	3386	0	3286	162	6
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6525	298	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 23.

All (298) 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: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:272:ILE:HG21	1:B:315:GLN:HE21	1.40	0.85
1:A:109:MET:HE1	1:A:123:MET:HB2	1.57	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:112:ASN:HB3	1:B:115:MET:HE3	1.58	0.83
1:B:335:SER:O	1:B:336:ASP:HB2	1.76	0.83
1:B:333:GLU:HG2	1:B:334:SER:N	1.87	0.82
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:O	1:B:337:ARG:HD3	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:A:455:LEU:C	1:A:457:VAL:H	1.98	0.71
1:B:67:VAL:HG13	1:B:89:LEU:HD11	1.73	0.70
1:B:7:TYR:CE1	1:B:47:ALA:HA	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:MET:HE3	1:B:102:ALA:HB3	1.74	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: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:26:CYS:HB3	1:B:123:MET:HE2	1.79	0.64
1:B:165:ILE:HG21	1:B:176:PHE:CE2	2.33	0.64
1:B:324:THR:O	1:B:325:MET:HB3	1.98	0.64
1:B:48:GLU:HB3	1:B:115:MET:HE1	1.80	0.63
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:A:104:PHE:CE2	1:A:311:MET:HE2	2.34	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:38:TYR:HE2	1:B:74:VAL:HG22	1.64	0.62
1:B:39:VAL:HG22	1:B:74:VAL:HG11	1.81	0.62
1:A:299:SER:HB2	1:B:301:ARG:NH1	2.15	0.62
1:A:95:THR:HB	1:B:239:GLU:OE1	1.99	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:HE1	1:B:123:MET:HB3	1.84	0.60
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:100:MET:CE	1:B:102:ALA:HB3	2.32	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:A:104:PHE:HE2	1:A:311:MET:HE2	1.70	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:HB3	1:A:354:ARG:CZ	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:18:ILE:HD11	4:A:626:HOH:O	2.06	0.55
1:A:172:ARG:HB3	1:A:173:PRO:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:C	1:A:457:VAL:N	2.65	0.55
1:B:8:VAL:HG23	1:B:43:ALA:HB2	1.88	0.55
1:B:295:THR:HG23	1:B:305:ALA:HB2	1.88	0.55
1:A:128:VAL:HG23	1:A:133:ARG:HB2	1.89	0.54
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: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:109:MET:HE2	1:B:302:GLY:O	2.09	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:130:GLU:CD	1:A:133:ARG:HH12	2.16	0.52
1:A:337:ARG:HB2	1:A:337:ARG:HH21	1.73	0.52
1:A:288:ARG:HD2	1:A:320:ILE:HD11	1.92	0.52
1:B:52:GLY:O	1:B:53:THR:CB	2.58	0.52
1:B:124:HIS:O	1:B:125:ASP:HB2	2.10	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:166:LYS:HA	1:B:167:PRO:C	2.36	0.51
1:B:304:THR:CG2	1:B:306:PHE:HB3	2.40	0.51
1:B:15:GLU:CD	1:B:15:GLU:H	2.18	0.51
1:A:107:LEU:HD13	1:B:195:PRO:HB3	1.93	0.51
1:A:288:ARG:HE	1:A:308:HIS:CD2	2.29	0.51
1:B:333:GLU:CG	1:B:334:SER:N	2.67	0.51
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:B:48:GLU:HB3	1:B:115:MET:CE	2.41	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:372:ASN:HD21	1:B:443:ASP:CG	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:PHE:CD1	1:B:403:PRO:HG3	2.48	0.49
1:A:146:LEU:HD12	1:A:146:LEU:N	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:33:LYS:O	1:B:36:TYR:HD1	1.96	0.48
1:B:222:THR:HG21	1:B:226:LYS:CE	2.43	0.48
1:B:142:ASN:ND2	1:B:361:LYS:HG2	2.28	0.48
1:B:361:LYS:HZ3	1:B:361:LYS:HB2	1.78	0.48
1:A:65:ARG:HD2	1:A:65:ARG:O	2.13	0.48
1:A:152:ARG:HB3	1:A:153:PRO:HD2	1.95	0.48
1:A:3:GLN:C	1:A:4:SER:O	2.54	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:B:8:VAL:CG2	1:B:43:ALA:HB2	2.43	0.48
1:A:120:TYR:HB2	1:A:300:LYS:O	2.13	0.48
1:A:10:LEU:O	1:A:11:ALA:CB	2.62	0.47
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:13:LYS:HB3	1:A:15:GLU:OE1	2.14	0.47
1:B:288:ARG:HH21	1:B:288:ARG:HD2	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:306:PHE:HZ	1:A:342:MET:HE3	1.80	0.47
1:B:425:ASP:CG	1:B:428:ARG:HH11	2.22	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:B:376:MET:HE2	1:B:380:PHE:CZ	2.49	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:A:122:LYS:HA	1:A:302:GLY:O	2.15	0.46
1:A:166:LYS:HA	1:A:167:PRO:C	2.41	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:447:ILE:C	1:B:449:PRO:HD3	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:CYS:SG	1:B:123:MET:HE2	2.56	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:101:ILE:O	1:B:102:ALA:C	2.58	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:337:ARG:HD3	1:B:337:ARG:C	2.41	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
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:A:109:MET:HE1	1:A:123:MET:CB	2.39	0.45
1:A:112:ASN:HA	1:A:115:MET:SD	2.57	0.45
1:A:4:SER:O	1:A:6:ARG:N	2.46	0.45
1:A:53:THR:HG22	1:A:54:ASN:N	2.32	0.45
1:A:376:MET:CB	1:A:377:PRO:HD3	2.45	0.45
1:B:321:HIS:HE1	1:B:324:THR:HG23	1.81	0.45
1:A:113:GLN:O	1:B:292:GLY:HA3	2.16	0.44
1:B:119:GLU:O	1:B:119:GLU:HG2	2.17	0.44
1:A:337:ARG:HB2	1:A:337:ARG:NH2	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:HD12	1:A:146:LEU:H	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:120:TYR:HB2	1:B:300:LYS:O	2.18	0.43
1:B:174:LYS:HB3	1:B:175:PRO:HD3	2.00	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:89:LEU:HD22	1:B:169:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PHE:HE2	1:A:311:MET:CE	2.31	0.43
1:B:109:MET:HE1	1:B:123:MET:CB	2.49	0.43
1:B:376:MET:HG3	1:B:380:PHE:CE2	2.53	0.43
1:B:26:CYS:CB	1:B:123:MET:HE2	2.45	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:A:3:GLN:OE1	1:A:3:GLN:N	2.48	0.42
1:A:25:LEU:HD23	4:A:626:HOH:O	2.19	0.42
1:A:199:GLN:HA	1:A:200:PRO:HD2	1.81	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
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: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:B:75:ASP:HA	1:B:76:GLU:OE2	2.21	0.41
1:B:176:PHE:CE1	1:B:211:VAL:HG21	2.56	0.41
1:A:296:SER:HA	1:A:297:PRO:HD3	1.86	0.41
1:A:448:TYR:O	1:A:449:PRO:C	2.63	0.41
1:B:74:VAL:HA	1:B:80:LEU:O	2.20	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:33:LYS:HG3	4:B:746:HOH:O	2.19	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: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:A:15:GLU:CD	1:A:15:GLU:H	2.27	0.41
1:A:112:ASN:C	1:A:112:ASN:HD22	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:TYR:CE2	1:B:291:HIS:HA	2.55	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: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:A:288:ARG:O	1:A:289:ALA:C	2.64	0.41
1:A:375:ARG:O	1:A:376:MET:C	2.64	0.41
1:B:45:PHE:CZ	1:B:112:ASN:HB2	2.55	0.41
1:B:143:ILE:HB	1:B:364:THR:HG21	2.03	0.41
1:B:152:ARG:CB	1:B:153:PRO:CD	2.96	0.41
1:B:305:ALA:O	1:B:306:PHE:C	2.64	0.41
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:A:155:VAL:O	1:A:156:ASP:HB2	2.21	0.41
1:A:204:LEU:C	1:A:204:LEU:HD23	2.46	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:B:448:TYR:O	1:B:449:PRO:C	2.64	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
4:A:631:HOH:O	4:B:569:HOH:O[1_545]	2.18	0.02
1:B:450:GLY:CA	4:B:833:HOH:O[2_645]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	1
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	1

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	274 (83%)	56 (17%)	2	2
1	B	334/376 (89%)	285 (85%)	49 (15%)	3	3
All	All	664/752 (88%)	559 (84%)	105 (16%)	2	2

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	GLN
1	A	5	SER
1	A	17	LEU
1	A	54	ASN
1	A	65	ARG
1	A	70	LEU
1	A	74	VAL
1	A	78	ARG
1	A	80	LEU
1	A	87	VAL
1	A	95	THR
1	A	107	LEU
1	A	111	ASN
1	A	112	ASN
1	A	113	GLN
1	A	135	LEU
1	A	142	ASN

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Mol	Chain	Res	Type
1	A	144	SER
1	A	165	ILE
1	A	166	LYS
1	A	168	LYS
1	A	169	LEU
1	A	171	LEU
1	A	172	ARG
1	A	174	LYS
1	A	175	PRO
1	A	178	GLU
1	A	191	LYS
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	294	VAL
1	A	300	LYS
1	A	313	ARG
1	A	322	THR
1	A	336	ASP
1	A	344	THR
1	A	347	GLU
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	404	VAL
1	A	410	LEU
1	A	418	ARG
1	A	424	LEU
1	A	448	TYR
1	A	449	PRO
1	A	451	TRP
1	B	15	GLU
1	B	54	ASN
1	B	67	VAL
1	B	74	VAL

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Mol	Chain	Res	Type
1	B	80	LEU
1	B	98	LYS
1	B	101	ILE
1	B	109	MET
1	B	111	ASN
1	B	112	ASN
1	B	115	MET
1	B	154	GLU
1	B	161	VAL
1	B	163	THR
1	B	164	ILE
1	B	169	LEU
1	B	172	ARG
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	291	HIS
1	B	295	THR
1	B	304	THR
1	B	322	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	361	LYS
1	B	367	ILE
1	B	376	MET
1	B	382	ASN
1	B	410	LEU
1	B	424	LEU
1	B	431	LYS
1	B	435	ARG

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Mol	Chain	Res	Type
1	B	449	PRO
1	B	455	LEU
1	B	457	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	112	ASN
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	124	HIS
1	B	142	ASN
1	B	287	HIS
1	B	298	GLN
1	B	308	HIS
1	B	315	GLN
1	B	349	GLN
1	B	382	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 oligosaccharides 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	-	-	-		
3	FOR	A	501	2,1	0,1,1	-	-	-		

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 [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.