



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 09:38 AM EST

PDB ID : 1RUS
Title : CRYSTAL STRUCTURE OF THE BINARY COMPLEX OF RIBULOSE-1, 5-BISPHOSPHATE CARBOXYLASE AND ITS PRODUCT, 3-PHOSPHO-D-GLYCERATE
Authors : Lundqvist, T.; Schneider, G.
Deposited on : 1991-10-10
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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 : 4.02b-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) : 2.36

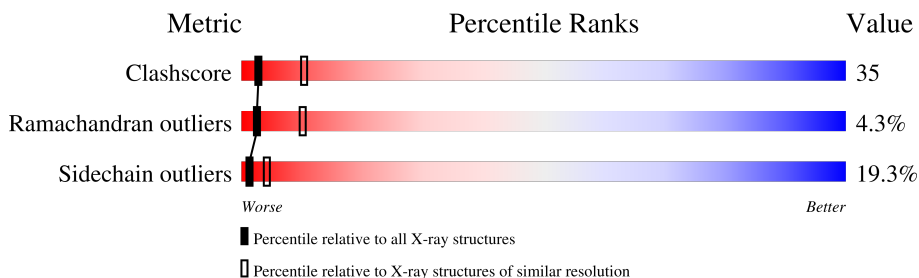
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3PG	A	500	-	X	X	-
2	3PG	B	500	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6677 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

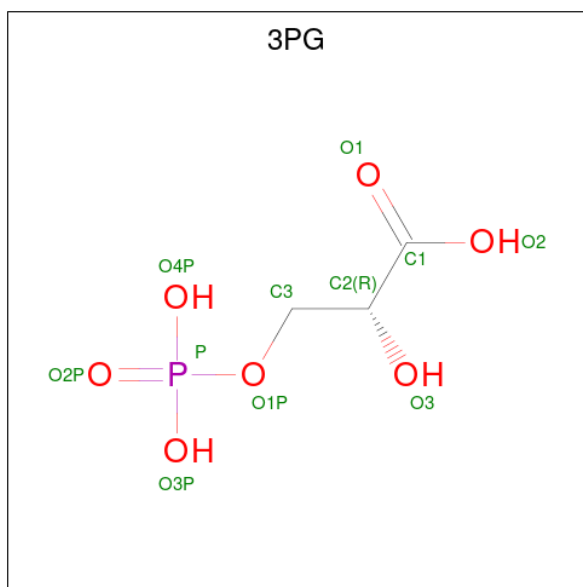
- Molecule 1 is a protein called RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	Total 3337	C 2115	N 589	O 617	S 16	7	0	0
1	B	435	Total 3318	C 2105	N 584	O 613	S 16	10	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 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: C₃H₇O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	Total 11	C 3	O 7	P 1	0	0

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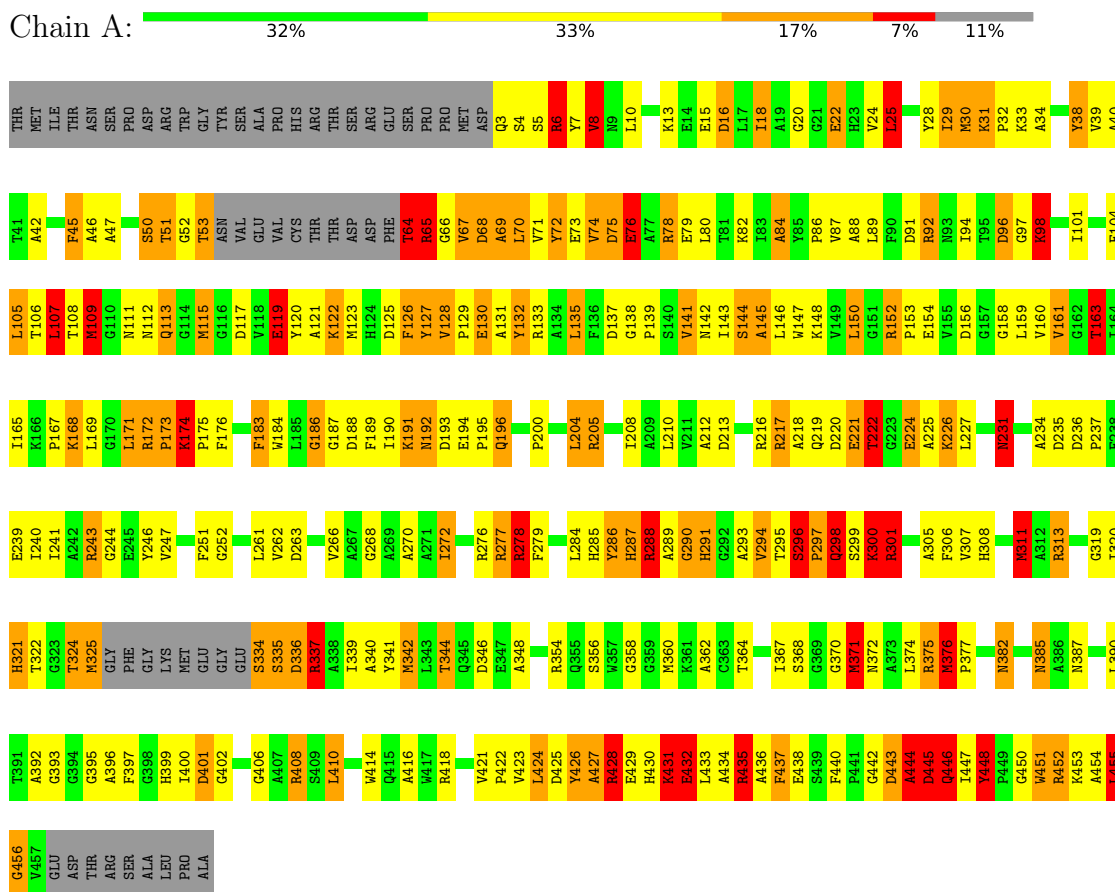
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	B	1	11	3	7	1	0	0

3 Residue-property plots [i](#)

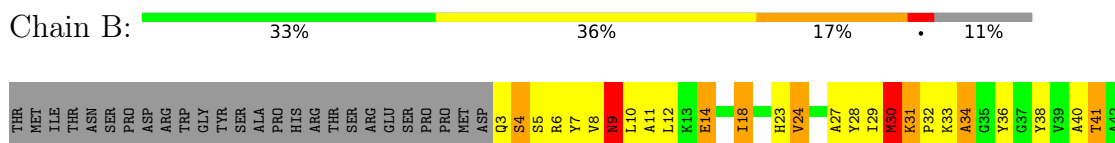
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

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



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



H399	A43	T106	EI78	F251	GLY	H399
I400	H44	L107	F183	N254	PHE	I400
D401	P45	L108	W184	H257	GLY	D401
R408	A46	M109	L185	L261	LYS	R408
S409	A47	G110	F189	Y265	GLU	S409
L410	E48	M111	I190	V266	GLY	L410
R411	S49	G112	K191	A267	S334	R411
R412	S50	M115	D192	G268	S335	R412
R413	T51	G116	D193	A269	D336	R413
R414	G52	D117	E194	A270	R387	R414
R418	ASN	V118	F195	A271	A338	R418
D419	VAL	E119	Q196	I272	I339	D419
P422	GLU	Y120	P200	T273	A340	P422
V423	VAL	A121	F201	T274	M342	V423
L424	CYS	D125	R206	R276	L343	L424
D425	THR	F126	D206	R277	T344	D425
R428	THR	Y127	I207	R278	Q345	R428
E429	THR	A131	I208	R279	A348	E429
H430	ASP	Y132	A209	L284	R354	H430
K431	ASP	R133	R210	H285	M360	K431
E432	ASP	D137	V211	Y286	R361	E432
L433	PHE	G138	A212	H287	A362	L433
A434	THR	P139	A214	R288	C363	A434
A436	THR	G140	M215	A289	T364	A436
F437	ARG	S140	R216	G290	P365	F437
E438	ARG	N142	R217	H291	I366	E438
S439	G66	K148	A218	G292	I367	S439
F440	V67	V149	Q219	A293	M371	F440
D443	D68	E79	D220	V294	N372	D443
A444	A69	L80	E221	T295	A373	A444
D445	L70	L150	T222	S296	L374	D445
Q446	E73	G151	G223	P297	R375	Q446
Y448	V74	R152	E224	Q298	M376	Y448
P449	D75	P153	R226	S299	P377	P449
G450	E76	D156	Q227	K300	G378	G450
R451	A77	G157	N231	G302	F379	R451
R452	R78	G158	I232	V307	F380	R452
K453	E79	L159	T233	H308	E381	K453
L454	L80	L160	A234	L383	N382	L454
G456	T81	V161	D235	G384	L384	G456
V457	K82	T163	E239	M385	M385	V457
GLU	R83	I164	I240	R313	A386	GLU
ASP	L94	I165	I241	L314	N387	ASP
THR	T95	K166	A242	Q315	T391	THR
ARG	D96	K168	R243	G316	A392	ARG
SER	G97	P169	G244	A317	G393	SER
ALA	K98	L169	E245	A317	G394	ALA
LEU	I101	R172	Y246	H321	G395	LEU
PRO	A102	P173	V247	T322	A396	PRO
ALA	S103	K174	T250	T324	F397	ALA
		P175		M325	G398	

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	65.50Å 70.60Å 104.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6677	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: 3PG

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	1.04	2/3417 (0.1%)	2.34	189/4629 (4.1%)
1	B	1.13	6/3398 (0.2%)	2.37	182/4604 (4.0%)
All	All	1.08	8/6815 (0.1%)	2.35	371/9233 (4.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	GLU	CD-OE1	-6.38	1.18	1.25
1	B	195	PRO	N-CD	-5.90	1.39	1.47
1	B	194	GLU	CG-CD	5.88	1.60	1.51
1	B	288	ARG	CD-NE	5.87	1.56	1.46
1	B	288	ARG	NE-CZ	5.71	1.40	1.33
1	A	432	GLU	CD-OE1	-5.29	1.19	1.25
1	A	438	GLU	CD-OE1	-5.20	1.20	1.25
1	B	194	GLU	CD-OE2	5.01	1.31	1.25

All (371) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ARG	NE-CZ-NH1	31.64	136.12	120.30
1	B	418	ARG	NE-CZ-NH1	29.99	135.30	120.30
1	B	418	ARG	CD-NE-CZ	23.09	155.92	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	429	GLU	CA-CB-CG	22.29	162.44	113.40
1	A	428	ARG	NE-CZ-NH1	21.75	131.17	120.30
1	B	152	ARG	NE-CZ-NH2	20.81	130.70	120.30
1	A	418	ARG	NE-CZ-NH2	-19.53	110.54	120.30
1	A	216	ARG	NE-CZ-NH2	-19.44	110.58	120.30
1	A	418	ARG	NE-CZ-NH1	19.24	129.92	120.30
1	A	6	ARG	NE-CZ-NH2	-18.63	110.99	120.30
1	A	172	ARG	NE-CZ-NH1	17.82	129.21	120.30
1	B	408	ARG	NE-CZ-NH2	-17.67	111.46	120.30
1	B	428	ARG	NE-CZ-NH2	16.32	128.46	120.30
1	A	428	ARG	CD-NE-CZ	16.23	146.32	123.60
1	B	205	ARG	NE-CZ-NH2	16.14	128.37	120.30
1	B	401	ASP	CB-CG-OD1	14.77	131.60	118.30
1	A	418	ARG	CD-NE-CZ	14.18	143.44	123.60
1	A	152	ARG	NE-CZ-NH2	13.04	126.82	120.30
1	B	443	ASP	CB-CG-OD1	12.85	129.87	118.30
1	A	16	ASP	CB-CG-OD2	-12.51	107.04	118.30
1	A	216	ARG	CD-NE-CZ	12.45	141.03	123.60
1	A	213	ASP	CB-CG-OD2	-12.27	107.26	118.30
1	A	133	ARG	NE-CZ-NH2	-12.13	114.23	120.30
1	B	133	ARG	NE-CZ-NH2	11.99	126.29	120.30
1	B	152	ARG	NE-CZ-NH1	-11.98	114.31	120.30
1	B	117	ASP	CB-CG-OD1	11.86	128.97	118.30
1	B	156	ASP	CB-CG-OD1	11.53	128.68	118.30
1	B	411	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	217	ARG	NE-CZ-NH2	-11.41	114.59	120.30
1	B	91	ASP	CB-CG-OD1	11.32	128.49	118.30
1	A	401	ASP	CB-CG-OD1	10.85	128.06	118.30
1	B	117	ASP	CA-CB-CG	10.72	136.99	113.40
1	B	408	ARG	NH1-CZ-NH2	10.48	130.93	119.40
1	A	432	GLU	CA-CB-CG	10.40	136.28	113.40
1	A	76	GLU	OE1-CD-OE2	-10.40	110.83	123.30
1	A	321	HIS	CB-CA-C	10.26	130.92	110.40
1	B	288	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	B	216	ARG	CD-NE-CZ	10.12	137.77	123.60
1	B	68	ASP	CB-CG-OD2	-10.09	109.22	118.30
1	A	76	GLU	CG-CD-OE1	10.00	138.30	118.30
1	B	445	ASP	CB-CG-OD1	9.90	127.21	118.30
1	B	96	ASP	CB-CG-OD2	9.87	127.18	118.30
1	A	25	LEU	CA-CB-CG	9.86	137.99	115.30
1	B	418	ARG	NH1-CZ-NH2	-9.85	108.57	119.40
1	B	435	ARG	NE-CZ-NH2	9.74	125.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	HIS	CA-CB-CG	9.73	130.14	113.60
1	B	419	ASP	CB-CG-OD2	9.46	126.81	118.30
1	B	67	VAL	N-CA-CB	9.25	131.84	111.50
1	A	75	ASP	CB-CG-OD2	-9.06	110.14	118.30
1	A	455	LEU	C-N-CA	8.97	141.14	122.30
1	A	428	ARG	CG-CD-NE	8.88	130.44	111.80
1	A	92	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	B	68	ASP	CB-CG-OD1	8.69	126.12	118.30
1	B	418	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	A	217	ARG	NH1-CZ-NH2	8.52	128.78	119.40
1	A	172	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	A	430	HIS	CA-CB-CG	-8.45	99.24	113.60
1	B	429	GLU	OE1-CD-OE2	-8.44	113.18	123.30
1	B	399	HIS	CA-CB-CG	8.32	127.74	113.60
1	B	110	GLY	CA-C-O	8.31	135.56	120.60
1	B	288	ARG	CD-NE-CZ	8.31	135.24	123.60
1	A	137	ASP	C-N-CA	8.30	139.72	122.30
1	B	127	TYR	CB-CG-CD1	8.28	125.97	121.00
1	A	52	GLY	C-N-CA	8.26	142.35	121.70
1	A	428	ARG	NH1-CZ-NH2	-8.23	110.35	119.40
1	A	91	ASP	CB-CG-OD1	8.21	125.68	118.30
1	A	144	SER	CA-CB-OG	8.18	133.28	111.20
1	B	428	ARG	NH1-CZ-NH2	-8.11	110.48	119.40
1	B	395	GLY	N-CA-C	-8.07	92.92	113.10
1	A	226	LYS	CB-CG-CD	8.06	132.54	111.60
1	A	188	ASP	CA-CB-CG	8.00	131.00	113.40
1	B	276	ARG	NE-CZ-NH2	7.99	124.29	120.30
1	A	454	ALA	C-N-CA	7.97	141.62	121.70
1	A	130	GLU	CB-CG-CD	7.95	135.65	114.20
1	A	226	LYS	CA-CB-CG	7.89	130.76	113.40
1	B	354	ARG	NE-CZ-NH2	7.87	124.24	120.30
1	A	163	THR	N-CA-CB	7.80	125.12	110.30
1	A	224	GLU	CB-CG-CD	7.78	135.20	114.20
1	A	64	THR	CA-CB-CG2	7.76	123.27	112.40
1	B	117	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	B	205	ARG	CA-CB-CG	7.75	130.46	113.40
1	B	201	PHE	CB-CG-CD2	7.72	126.20	120.80
1	B	28	TYR	CG-CD2-CE2	7.69	127.45	121.30
1	A	213	ASP	CB-CG-OD1	7.68	125.22	118.30
1	B	401	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	B	48	GLU	CA-C-N	7.62	133.95	117.20
1	A	437	PHE	C-N-CA	7.61	140.72	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	GLU	CA-CB-CG	7.57	130.06	113.40
1	A	425	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	24	VAL	CA-C-N	7.57	133.84	117.20
1	A	217	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	A	171	LEU	O-C-N	-7.52	110.67	122.70
1	B	213	ASP	CB-CG-OD1	7.46	125.01	118.30
1	B	110	GLY	N-CA-C	7.44	131.70	113.10
1	B	79	GLU	OE1-CD-OE2	-7.42	114.40	123.30
1	A	337	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	127	TYR	CB-CG-CD2	-7.38	116.58	121.00
1	A	156	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	426	TYR	CB-CG-CD1	-7.30	116.62	121.00
1	A	220	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	325	MET	CG-SD-CE	7.29	111.86	100.20
1	A	133	ARG	NH1-CZ-NH2	7.25	127.38	119.40
1	A	313	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	A	28	TYR	CA-CB-CG	7.23	127.14	113.40
1	B	79	GLU	CG-CD-OE1	7.17	132.63	118.30
1	B	28	TYR	CA-CB-CG	7.15	126.99	113.40
1	B	150	LEU	C-N-CA	7.05	137.10	122.30
1	B	45	PHE	CA-CB-CG	7.02	130.74	113.90
1	A	425	ASP	CB-CA-C	7.02	124.43	110.40
1	B	94	ILE	CA-CB-CG1	7.00	124.31	111.00
1	A	429	GLU	CG-CD-OE1	7.00	132.29	118.30
1	A	51	THR	CA-C-N	6.99	130.17	116.20
1	A	16	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	29	ILE	CB-CA-C	6.97	125.55	111.60
1	A	277	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	276	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	A	98	LYS	CD-CE-NZ	6.95	127.68	111.70
1	B	207	THR	CA-CB-OG1	-6.94	94.42	109.00
1	A	38	TYR	CB-CG-CD1	6.93	125.16	121.00
1	B	337	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	A	84	ALA	C-N-CA	6.91	138.98	121.70
1	A	6	ARG	NH1-CZ-NH2	6.89	126.98	119.40
1	B	148	LYS	CA-C-N	6.86	132.30	117.20
1	A	186	GLY	C-N-CA	6.86	136.71	122.30
1	A	451	TRP	N-CA-CB	-6.85	98.28	110.60
1	B	125	ASP	CB-CG-OD1	6.83	124.44	118.30
1	A	174	LYS	CA-CB-CG	6.82	128.41	113.40
1	B	219	GLN	N-CA-CB	6.81	122.86	110.60
1	A	130	GLU	OE1-CD-OE2	-6.81	115.13	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	MET	CG-SD-CE	6.81	111.09	100.20
1	A	205	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	216	ARG	CG-CD-NE	6.75	125.99	111.80
1	B	130	GLU	CG-CD-OE1	6.75	131.81	118.30
1	A	152	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
1	B	95	THR	O-C-N	-6.75	111.90	122.70
1	B	445	ASP	CA-CB-CG	6.73	128.21	113.40
1	B	31	LYS	CA-CB-CG	6.72	128.18	113.40
1	B	452	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	A	128	VAL	CA-CB-CG1	6.69	120.94	110.90
1	A	145	ALA	CB-CA-C	6.68	120.12	110.10
1	B	313	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	A	444	ALA	CA-C-N	6.66	131.85	117.20
1	A	278	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	B	96	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	A	91	ASP	CB-CA-C	6.62	123.64	110.40
1	B	277	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	456	GLY	CA-C-O	6.58	132.45	120.60
1	B	89	LEU	CA-CB-CG	6.58	130.44	115.30
1	B	428	ARG	CG-CD-NE	6.58	125.61	111.80
1	B	91	ASP	CA-CB-CG	6.57	127.86	113.40
1	B	115	MET	CG-SD-CE	6.57	110.71	100.20
1	B	278	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	B	93	ASN	CA-CB-CG	6.56	127.82	113.40
1	B	48	GLU	N-CA-CB	6.55	122.40	110.60
1	B	226	LYS	CA-CB-CG	6.55	127.82	113.40
1	B	118	VAL	C-N-CA	6.55	138.07	121.70
1	B	108	THR	C-N-CA	6.55	138.07	121.70
1	A	138	GLY	CA-C-O	-6.54	108.82	120.60
1	A	452	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	24	VAL	O-C-N	-6.52	112.27	122.70
1	A	38	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	A	112	ASN	CA-C-O	6.51	133.77	120.10
1	A	410	LEU	CA-CB-CG	6.50	130.25	115.30
1	B	288	ARG	NH1-CZ-NH2	-6.49	112.26	119.40
1	A	301	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	B	30	MET	N-CA-CB	6.47	122.25	110.60
1	A	96	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	221	GLU	CG-CD-OE1	6.45	131.19	118.30
1	A	222	THR	N-CA-CB	-6.43	98.08	110.30
1	A	76	GLU	CB-CG-CD	6.40	131.48	114.20
1	B	394	GLY	CA-C-O	6.39	132.11	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	LEU	CA-CB-CG	6.39	130.00	115.30
1	A	22	GLU	CG-CD-OE1	6.39	131.07	118.30
1	A	75	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	97	GLY	C-N-CA	6.38	137.64	121.70
1	A	296	SER	N-CA-CB	-6.36	100.96	110.50
1	A	183	PHE	N-CA-CB	6.34	122.02	110.60
1	B	14	GLU	CG-CD-OE2	-6.34	105.63	118.30
1	B	48	GLU	CA-C-O	-6.33	106.80	120.10
1	A	435	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	133	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	147	TRP	N-CA-CB	6.30	121.93	110.60
1	A	53	THR	CA-C-O	-6.28	106.92	120.10
1	A	145	ALA	N-CA-CB	-6.28	101.31	110.10
1	B	91	ASP	OD1-CG-OD2	-6.25	111.42	123.30
1	A	445	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	126	PHE	CA-CB-CG	6.22	128.82	113.90
1	A	212	ALA	CB-CA-C	6.16	119.34	110.10
1	B	95	THR	C-N-CA	6.16	137.10	121.70
1	A	189	PHE	N-CA-CB	-6.14	99.54	110.60
1	B	216	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	220	ASP	OD1-CG-OD2	-6.12	111.66	123.30
1	A	342	MET	CG-SD-CE	6.12	109.99	100.20
1	A	42	ALA	CB-CA-C	6.12	119.27	110.10
1	B	66	GLY	O-C-N	6.11	132.47	122.70
1	A	79	GLU	CA-CB-CG	6.10	126.83	113.40
1	B	311	MET	CG-SD-CE	6.10	109.97	100.20
1	B	73	GLU	CA-C-O	6.09	132.89	120.10
1	B	73	GLU	CA-CB-CG	6.09	126.79	113.40
1	B	126	PHE	CA-CB-CG	6.09	128.51	113.90
1	A	375	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	144	SER	CB-CA-C	6.07	121.64	110.10
1	A	360	MET	CG-SD-CE	6.07	109.92	100.20
1	B	342	MET	CG-SD-CE	6.07	109.92	100.20
1	A	288	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	B	207	THR	CA-CB-CG2	6.06	120.88	112.40
1	A	38	TYR	N-CA-CB	6.05	121.49	110.60
1	B	12	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	217	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	9	ASN	N-CA-CB	6.01	121.41	110.60
1	A	112	ASN	O-C-N	-5.99	113.12	122.70
1	A	72	TYR	CB-CG-CD2	5.98	124.59	121.00
1	A	160	VAL	CG1-CB-CG2	-5.98	101.33	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	PHE	O-C-N	-5.97	113.15	122.70
1	B	409	SER	C-N-CA	5.97	136.62	121.70
1	A	45	PHE	CB-CA-C	5.96	122.33	110.40
1	A	451	TRP	CB-CG-CD2	-5.94	118.88	126.60
1	B	41	THR	C-N-CA	5.94	136.56	121.70
1	B	152	ARG	CD-NE-CZ	-5.92	115.32	123.60
1	A	287	HIS	O-C-N	-5.90	113.25	122.70
1	A	188	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	82	LYS	CG-CD-CE	5.89	129.56	111.90
1	B	447	ILE	CB-CA-C	5.89	123.37	111.60
1	A	112	ASN	CB-CA-C	5.88	122.17	110.40
1	B	221	GLU	CB-CG-CD	5.88	130.06	114.20
1	B	166	LYS	CA-CB-CG	-5.87	100.48	113.40
1	A	67	VAL	CB-CA-C	5.85	122.52	111.40
1	A	137	ASP	N-CA-CB	-5.85	100.07	110.60
1	A	15	GLU	OE1-CD-OE2	5.85	130.31	123.30
1	B	48	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	A	354	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	141	VAL	CA-CB-CG1	5.81	119.61	110.90
1	B	73	GLU	O-C-N	-5.80	113.42	122.70
1	A	220	ASP	O-C-N	-5.79	113.44	122.70
1	A	427	ALA	N-CA-CB	5.79	118.20	110.10
1	A	376	MET	CG-SD-CE	5.79	109.46	100.20
1	B	36	TYR	CB-CG-CD1	5.76	124.46	121.00
1	B	85	TYR	CB-CG-CD1	5.76	124.45	121.00
1	A	220	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	120	TYR	CA-C-N	-5.75	104.56	117.20
1	A	172	ARG	CD-NE-CZ	5.74	131.63	123.60
1	B	115	MET	CB-CA-C	5.74	121.88	110.40
1	B	24	VAL	CA-C-O	-5.74	108.06	120.10
1	B	14	GLU	CG-CD-OE1	5.72	129.74	118.30
1	B	121	ALA	CB-CA-C	5.72	118.67	110.10
1	B	397	PHE	C-N-CA	5.69	134.25	122.30
1	A	448	TYR	CA-CB-CG	5.69	124.21	113.40
1	B	97	GLY	C-N-CA	5.69	135.92	121.70
1	A	430	HIS	CA-C-O	5.68	132.03	120.10
1	A	73	GLU	CA-C-O	5.68	132.02	120.10
1	B	205	ARG	NH1-CZ-NH2	-5.67	113.17	119.40
1	B	40	ALA	N-CA-CB	-5.66	102.17	110.10
1	A	133	ARG	CD-NE-CZ	-5.66	115.67	123.60
1	A	65	ARG	N-CA-CB	5.66	120.78	110.60
1	A	219	GLN	CB-CG-CD	5.65	126.30	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	B	428	ARG	CD-NE-CZ	5.65	131.50	123.60
1	B	80	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	B	77	ALA	CB-CA-C	5.62	118.54	110.10
1	A	8	VAL	CA-C-O	-5.62	108.29	120.10
1	A	115	MET	CG-SD-CE	5.62	109.19	100.20
1	A	440	PHE	CA-CB-CG	5.61	127.36	113.90
1	B	448	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	B	137	ASP	CA-C-N	5.60	127.40	116.20
1	B	166	LYS	CB-CA-C	5.60	121.59	110.40
1	A	371	MET	CG-SD-CE	5.58	109.13	100.20
1	A	131	ALA	N-CA-CB	-5.58	102.29	110.10
1	B	376	MET	CG-SD-CE	5.58	109.12	100.20
1	A	173	PRO	C-N-CA	5.57	135.63	121.70
1	A	444	ALA	CB-CA-C	5.57	118.46	110.10
1	B	24	VAL	CG1-CB-CG2	-5.57	101.99	110.90
1	B	52	GLY	CA-C-O	5.57	130.63	120.60
1	B	44	HIS	CB-CA-C	5.57	121.54	110.40
1	B	447	ILE	CA-CB-CG2	5.57	122.03	110.90
1	A	160	VAL	CA-CB-CG2	5.56	119.24	110.90
1	A	444	ALA	CA-C-O	-5.56	108.43	120.10
1	A	127	TYR	C-N-CA	5.55	135.57	121.70
1	A	216	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
1	A	152	ARG	O-C-N	5.55	131.64	121.10
1	A	75	ASP	N-CA-CB	5.54	120.58	110.60
1	A	212	ALA	C-N-CA	5.54	135.54	121.70
1	A	78	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	107	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	167	PRO	O-C-N	5.50	131.50	122.70
1	B	43	ALA	CB-CA-C	5.50	118.34	110.10
1	B	408	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	B	24	VAL	CA-C-N	5.48	129.25	117.20
1	A	3	GLN	O-C-N	5.46	131.44	122.70
1	A	68	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	138	GLY	O-C-N	5.45	131.46	121.10
1	A	224	GLU	OE1-CD-OE2	-5.45	116.77	123.30
1	B	27	ALA	CB-CA-C	5.44	118.25	110.10
1	A	18	ILE	C-N-CA	5.43	135.28	121.70
1	B	408	ARG	C-N-CA	5.43	135.28	121.70
1	B	278	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	B	38	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	443	ASP	CB-CG-OD2	-5.40	113.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	LEU	CB-CA-C	5.40	120.46	110.20
1	A	130	GLU	CB-CA-C	-5.40	99.60	110.40
1	B	114	GLY	CA-C-O	5.40	130.32	120.60
1	B	28	TYR	CD1-CE1-CZ	5.38	124.64	119.80
1	B	156	ASP	OD1-CG-OD2	-5.38	113.08	123.30
1	A	22	GLU	OE1-CD-OE2	-5.37	116.85	123.30
1	B	130	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	B	115	MET	C-N-CA	5.36	133.55	122.30
1	B	75	ASP	N-CA-C	-5.35	96.56	111.00
1	B	439	SER	CB-CA-C	-5.35	99.94	110.10
1	B	30	MET	CA-CB-CG	5.34	122.38	113.30
1	B	440	PHE	N-CA-CB	5.33	120.20	110.60
1	B	278	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	210	LEU	CA-CB-CG	5.32	127.55	115.30
1	A	25	LEU	CB-CG-CD2	5.32	120.05	111.00
1	A	325	MET	CG-SD-CE	5.31	108.70	100.20
1	A	52	GLY	CA-C-O	5.31	130.16	120.60
1	B	90	PHE	CB-CA-C	5.29	120.99	110.40
1	B	438	GLU	CA-C-O	-5.29	109.00	120.10
1	B	29	ILE	CA-CB-CG2	5.28	121.46	110.90
1	A	158	GLY	N-CA-C	5.28	126.29	113.10
1	B	213	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	225	ALA	CB-CA-C	5.25	117.98	110.10
1	B	110	GLY	C-N-CA	5.24	134.80	121.70
1	A	150	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	149	VAL	CA-CB-CG1	5.24	118.76	110.90
1	B	194	GLU	OE1-CD-OE2	-5.23	117.03	123.30
1	B	139	PRO	CB-CA-C	5.22	125.05	112.00
1	A	231	ASN	O-C-N	5.21	131.04	122.70
1	A	92	ARG	CA-C-O	-5.21	109.17	120.10
1	B	215	MET	N-CA-CB	5.21	119.97	110.60
1	B	360	MET	CG-SD-CE	5.20	108.52	100.20
1	B	133	ARG	CA-CB-CG	5.20	124.83	113.40
1	A	221	GLU	CA-C-O	5.19	131.01	120.10
1	B	148	LYS	CA-C-O	-5.19	109.20	120.10
1	A	125	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	429	GLU	CG-CD-OE1	5.18	128.67	118.30
1	A	98	LYS	CA-C-O	5.17	130.97	120.10
1	A	109	MET	CG-SD-CE	5.17	108.48	100.20
1	B	301	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	78	ARG	CD-NE-CZ	-5.15	116.39	123.60
1	B	221	GLU	CG-CD-OE2	-5.13	108.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ARG	CA-CB-CG	5.13	124.69	113.40
1	B	436	ALA	N-CA-CB	5.13	117.28	110.10
1	A	66	GLY	N-CA-C	-5.12	100.29	113.10
1	A	424	LEU	CB-CA-C	5.12	119.94	110.20
1	A	40	ALA	CB-CA-C	5.12	117.78	110.10
1	B	393	GLY	O-C-N	5.12	131.90	123.20
1	A	221	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	B	150	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	B	116	GLY	N-CA-C	-5.09	100.37	113.10
1	A	13	LYS	CA-CB-CG	5.09	124.59	113.40
1	B	297	PRO	O-C-N	5.08	130.84	122.70
1	B	110	GLY	O-C-N	-5.08	114.57	122.70
1	A	69	ALA	N-CA-CB	5.08	117.21	110.10
1	A	89	LEU	C-N-CA	5.08	134.39	121.70
1	A	160	VAL	N-CA-CB	5.08	122.67	111.50
1	B	27	ALA	CA-C-O	5.08	130.76	120.10
1	B	98	LYS	CB-CA-C	-5.07	100.27	110.40
1	A	428	ARG	CB-CA-C	5.07	120.53	110.40
1	B	28	TYR	CG-CD1-CE1	-5.06	117.25	121.30
1	A	448	TYR	CB-CA-C	-5.06	100.28	110.40
1	A	73	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	B	111	ASN	C-N-CA	5.05	134.33	121.70
1	B	18	ILE	C-N-CA	5.05	134.32	121.70
1	A	414	TRP	N-CA-CB	5.05	119.68	110.60
1	A	422	PRO	N-CA-C	-5.04	98.98	112.10
1	B	166	LYS	CB-CG-CD	5.04	124.72	111.60
1	B	96	ASP	C-N-CA	5.04	132.89	122.30
1	B	11	ALA	O-C-N	5.04	130.76	122.70
1	A	25	LEU	CB-CA-C	5.02	119.74	110.20
1	A	86	PRO	O-C-N	5.02	130.73	122.70
1	A	132	TYR	N-CA-CB	5.01	119.62	110.60
1	B	212	ALA	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	ASN	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	3337	0	3242	258	2
1	B	3318	0	3220	237	0
2	A	11	0	4	7	0
2	B	11	0	4	5	0
All	All	6677	0	6470	464	2

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 35.

All (464) 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:196:GLN:O	1:A:231:ASN:ND2	1.67	1.28
1:A:288:ARG:HD3	1:A:291:HIS:NE2	1.52	1.23
1:B:3:GLN:NE2	1:B:44:HIS:HA	1.50	1.22
1:B:321:HIS:HB3	2:B:500:3PG:O4P	1.41	1.17
1:B:335:SER:O	1:B:339:ILE:CG1	1.93	1.14
1:A:263:ASP:OD1	1:A:289:ALA:HB2	1.49	1.13
1:B:335:SER:O	1:B:339:ILE:HG13	0.97	1.12
1:A:194:GLU:HG3	1:A:195:PRO:HD3	1.17	1.11
1:A:334:SER:O	1:A:335:SER:HB3	1.53	1.08
1:A:293:ALA:O	1:A:299:SER:CB	2.03	1.06
1:B:324:THR:HG22	1:B:325:MET:H	1.19	1.06
1:B:335:SER:C	1:B:339:ILE:HG13	1.74	1.06
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.36	1.06
1:A:194:GLU:HG3	1:A:195:PRO:CD	1.85	1.05
1:A:288:ARG:HD3	1:A:291:HIS:HE2	0.96	1.04
1:A:293:ALA:HB2	1:B:301:ARG:HB2	1.40	1.03
1:A:194:GLU:CG	1:A:195:PRO:HD3	1.91	0.99
1:B:324:THR:CG2	1:B:325:MET:N	2.28	0.96
1:B:93:ASN:HD22	1:B:96:ASP:HB2	1.32	0.94
1:A:293:ALA:O	1:A:299:SER:OG	1.86	0.94
1:A:376:MET:HB3	1:A:377:PRO:HD3	1.49	0.93
1:B:324:THR:HG22	1:B:325:MET:N	1.80	0.91
1:A:324:THR:HG23	1:A:368:SER:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:HIS:CD2	1:A:291:HIS:H	1.60	0.91
1:B:321:HIS:CB	2:B:500:3PG:O4P	2.18	0.90
1:A:65:ARG:HG3	1:A:67:VAL:HG23	1.53	0.89
1:A:278:ARG:HE	1:A:278:ARG:HA	1.39	0.87
1:B:222:THR:HG23	1:B:224:GLU:HB2	1.56	0.87
1:A:288:ARG:HD3	1:A:291:HIS:CE1	2.10	0.86
1:A:291:HIS:CD2	1:A:291:HIS:N	2.41	0.86
1:B:241:ILE:HG12	1:B:278:ARG:HG2	1.58	0.85
1:A:289:ALA:O	1:B:111:ASN:N	2.10	0.84
1:A:344:THR:HA	1:A:362:ALA:HB1	1.58	0.84
1:A:163:THR:HG23	1:A:397:PHE:CE1	2.12	0.84
1:B:3:GLN:OE1	1:B:47:ALA:CB	2.26	0.83
1:B:291:HIS:CD2	1:B:295:THR:HG21	2.14	0.83
1:A:163:THR:HG23	1:A:397:PHE:HE1	1.42	0.82
1:A:263:ASP:OD1	1:A:289:ALA:CB	2.28	0.81
1:B:372:ASN:HD22	1:B:374:LEU:H	1.29	0.80
1:A:293:ALA:HB2	1:B:301:ARG:CB	2.11	0.80
1:A:401:ASP:OD2	1:A:435:ARG:HG2	1.84	0.78
1:B:3:GLN:NE2	1:B:44:HIS:CA	2.43	0.78
1:A:218:ALA:O	1:A:222:THR:HB	1.84	0.77
1:B:3:GLN:HE21	1:B:44:HIS:HA	1.49	0.77
1:B:376:MET:HB3	1:B:377:PRO:HD3	1.67	0.77
1:B:128:VAL:HG23	1:B:133:ARG:HB2	1.67	0.76
1:B:45:PHE:HA	1:B:115:MET:HE3	1.66	0.76
1:A:53:THR:HA	1:B:167:PRO:HB3	1.68	0.76
1:B:162:GLY:HA2	1:B:189:PHE:O	1.85	0.76
1:B:174:LYS:HB3	1:B:175:PRO:HD3	1.67	0.76
1:B:274:THR:O	1:B:278:ARG:HB3	1.86	0.75
1:A:392:ALA:HB1	1:A:396:ALA:HB3	1.68	0.75
1:B:399:HIS:CE1	1:B:401:ASP:HB2	2.22	0.75
1:A:285:HIS:NE2	1:A:321:HIS:CD2	2.55	0.74
1:B:31:LYS:O	1:B:119:GLU:HB2	1.85	0.74
1:A:105:LEU:HD23	1:A:109:MET:HE3	1.71	0.73
1:B:96:ASP:HB3	1:B:98:LYS:HG3	1.71	0.73
1:A:167:PRO:HB3	1:B:53:THR:HG22	1.69	0.73
1:B:74:VAL:HA	1:B:80:LEU:O	1.87	0.73
1:B:30:MET:HG2	1:B:31:LYS:N	2.03	0.73
1:B:3:GLN:HE21	1:B:44:HIS:CB	2.01	0.72
1:A:334:SER:O	1:A:335:SER:CB	2.30	0.72
1:B:372:ASN:ND2	1:B:374:LEU:HB2	2.04	0.72
1:B:456:GLY:O	1:B:457:VAL:HB	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLY:O	1:B:117:ASP:HB3	1.89	0.72
1:A:263:ASP:CG	1:A:289:ALA:HB2	2.10	0.72
1:A:268:GLY:HA3	1:B:268:GLY:HA3	1.70	0.72
1:A:385:ASN:HD22	1:A:387:ASN:H	1.37	0.72
1:B:376:MET:HB3	1:B:377:PRO:CD	2.20	0.71
1:A:107:LEU:HD13	1:B:195:PRO:HB3	1.72	0.71
1:A:370:GLY:HA3	1:A:396:ALA:HB2	1.72	0.71
1:A:368:SER:CB	2:A:500:3PG:O2P	2.38	0.71
1:B:14:GLU:O	1:B:18:ILE:HG13	1.90	0.71
1:A:400:ILE:HD11	1:A:435:ARG:HG3	1.71	0.71
1:B:290:GLY:O	1:B:292:GLY:N	2.23	0.71
1:A:174:LYS:HB3	1:A:175:PRO:HD3	1.72	0.71
1:B:321:HIS:ND1	2:B:500:3PG:O4P	2.23	0.71
1:A:168:LYS:HE3	1:A:193:ASP:OD1	1.91	0.70
1:B:183:PHE:HB3	1:B:190:ILE:HD11	1.72	0.70
1:B:234:ALA:HB3	1:B:240:ILE:HG13	1.73	0.70
1:A:321:HIS:HB3	2:A:500:3PG:O3P	1.91	0.70
1:A:152:ARG:HB3	1:A:153:PRO:HD2	1.73	0.69
1:A:296:SER:CB	1:A:297:PRO:HD2	2.22	0.69
1:A:286:TYR:HB3	1:A:320:ILE:HG13	1.74	0.69
1:B:3:GLN:OE1	1:B:47:ALA:HB2	1.91	0.69
1:A:191:LYS:O	1:A:191:LYS:HG3	1.92	0.69
1:A:293:ALA:HA	1:B:301:ARG:HD3	1.75	0.69
1:B:192:ASN:ND2	1:B:196:GLN:OE1	2.24	0.69
1:B:285:HIS:HE2	1:B:321:HIS:CD2	2.10	0.69
1:A:278:ARG:CG	1:A:279:PHE:CE1	2.76	0.69
1:A:96:ASP:HB3	1:A:98:LYS:HB2	1.74	0.68
1:A:70:LEU:H	1:A:70:LEU:HD12	1.58	0.68
1:A:431:LYS:O	1:A:434:ALA:HB3	1.94	0.68
1:B:301:ARG:HH11	1:B:301:ARG:HG2	1.59	0.68
1:A:299:SER:C	1:A:301:ARG:H	1.97	0.68
1:A:167:PRO:HB3	1:B:53:THR:HA	1.76	0.68
1:B:32:PRO:CB	1:B:41:THR:HG21	2.21	0.68
1:A:237:PRO:O	1:A:241:ILE:HG13	1.94	0.67
1:A:295:THR:HG23	1:A:305:ALA:N	2.08	0.67
1:A:376:MET:HB3	1:A:377:PRO:CD	2.25	0.67
1:A:278:ARG:HG3	1:A:279:PHE:CE1	2.29	0.66
1:A:342:MET:HA	1:A:348:ALA:CB	2.26	0.66
1:B:321:HIS:CG	2:B:500:3PG:O4P	2.48	0.66
1:A:370:GLY:CA	1:A:396:ALA:HB2	2.25	0.66
1:B:278:ARG:HD3	1:B:278:ARG:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASP:O	1:B:270:ALA:HA	1.95	0.66
1:B:374:LEU:HD11	1:B:437:PHE:HA	1.77	0.66
1:A:293:ALA:O	1:A:299:SER:HB3	1.92	0.66
1:A:289:ALA:O	1:B:111:ASN:CA	2.44	0.65
1:A:368:SER:HB3	2:A:500:3PG:O2P	1.96	0.65
1:A:65:ARG:HD2	1:A:65:ARG:O	1.96	0.65
1:A:288:ARG:CD	1:A:291:HIS:CE1	2.79	0.65
1:A:291:HIS:HB2	1:A:295:THR:HB	1.79	0.64
1:A:294:VAL:HG12	1:A:295:THR:N	2.12	0.64
1:A:392:ALA:HB3	1:A:397:PHE:CZ	2.32	0.64
1:A:142:ASN:OD1	1:A:144:SER:HB3	1.98	0.64
1:A:423:VAL:HG13	1:A:433:LEU:HD21	1.80	0.64
1:A:368:SER:HB2	2:A:500:3PG:O2P	1.97	0.64
1:B:93:ASN:HD22	1:B:96:ASP:CB	2.08	0.64
1:B:174:LYS:CB	1:B:175:PRO:HD3	2.28	0.64
1:A:217:ARG:O	1:A:221:GLU:HG3	1.97	0.64
1:B:335:SER:C	1:B:339:ILE:CG1	2.54	0.64
1:A:288:ARG:CD	1:A:291:HIS:HE2	1.91	0.63
1:A:291:HIS:CB	1:A:295:THR:HB	2.28	0.63
1:B:165:ILE:HG12	1:B:190:ILE:HG23	1.79	0.63
1:B:215:MET:O	1:B:219:GLN:HG3	1.98	0.63
1:A:222:THR:HG22	1:A:224:GLU:H	1.64	0.63
1:B:399:HIS:ND1	1:B:401:ASP:HB2	2.14	0.63
1:B:376:MET:HG3	1:B:380:PHE:CE2	2.33	0.63
1:A:107:LEU:HD13	1:B:195:PRO:CB	2.28	0.63
1:B:239:GLU:OE1	1:B:243:ARG:NE	2.32	0.62
1:A:167:PRO:HB3	1:B:53:THR:CG2	2.30	0.62
1:A:120:TYR:HB2	1:A:300:LYS:HB2	1.80	0.62
1:B:336:ASP:HA	1:B:339:ILE:HB	1.80	0.62
1:A:53:THR:CA	1:B:167:PRO:HB3	2.30	0.62
1:A:53:THR:O	1:B:166:LYS:HG2	2.00	0.62
1:B:178:GLU:OE1	1:B:217:ARG:NH2	2.26	0.62
1:A:278:ARG:HG3	1:A:279:PHE:CD1	2.34	0.61
1:B:3:GLN:HE22	1:B:44:HIS:HA	1.59	0.61
1:A:340:ALA:O	1:A:344:THR:OG1	2.19	0.61
1:B:67:VAL:O	1:B:89:LEU:HD21	2.01	0.61
1:A:150:LEU:HG	1:A:227:LEU:HD11	1.83	0.61
1:A:424:LEU:HD13	1:A:437:PHE:CZ	2.34	0.61
1:A:296:SER:C	1:A:298:GLN:H	2.04	0.61
1:A:278:ARG:HG2	1:A:279:PHE:CE1	2.36	0.60
1:B:371:MET:HB3	1:B:376:MET:HE1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:O	1:B:251:PHE:HD1	1.84	0.60
1:B:159:LEU:HD22	1:B:380:PHE:HZ	1.66	0.60
1:A:70:LEU:HD12	1:A:70:LEU:N	2.17	0.60
1:B:110:GLY:O	1:B:113:GLN:HB2	2.01	0.60
1:B:4:SER:O	1:B:6:ARG:N	2.35	0.60
1:A:122:LYS:NZ	1:A:294:VAL:O	2.35	0.60
1:A:270:ALA:HA	1:B:235:ASP:O	2.01	0.60
1:B:324:THR:O	1:B:325:MET:O	2.20	0.59
1:B:447:ILE:HD12	1:B:447:ILE:O	2.02	0.59
1:A:443:ASP:O	1:A:447:ILE:HG13	2.03	0.59
1:A:293:ALA:CB	1:B:301:ARG:HB2	2.25	0.59
1:A:46:ALA:O	1:A:50:SER:HB2	2.02	0.59
1:B:129:PRO:HG2	1:B:132:TYR:HB3	1.83	0.59
1:B:168:LYS:HE2	1:B:193:ASP:OD2	2.02	0.59
1:A:442:GLY:O	1:A:446:GLN:NE2	2.30	0.59
1:B:241:ILE:O	1:B:245:GLU:HG3	2.03	0.59
1:B:424:LEU:HD21	1:B:451:TRP:HA	1.85	0.58
1:A:167:PRO:CB	1:B:53:THR:HG22	2.31	0.58
1:A:270:ALA:HB3	1:B:270:ALA:HB3	1.85	0.58
1:A:120:TYR:CB	1:A:300:LYS:HB2	2.33	0.58
1:A:382:ASN:C	1:A:382:ASN:HD22	2.06	0.58
1:B:457:VAL:HG12	1:B:457:VAL:O	2.02	0.58
1:B:301:ARG:HG2	1:B:301:ARG:NH1	2.18	0.58
1:B:32:PRO:HB3	1:B:41:THR:CG2	2.22	0.58
1:A:397:PHE:HE2	1:A:410:LEU:CD1	2.16	0.58
1:B:3:GLN:HE21	1:B:44:HIS:HB2	1.67	0.57
1:B:424:LEU:HD23	1:B:454:ALA:HB3	1.85	0.57
1:B:393:GLY:O	1:B:397:PHE:HB2	2.03	0.57
1:B:424:LEU:HD11	1:B:448:TYR:HB3	1.86	0.57
1:A:234:ALA:HB3	1:A:240:ILE:HG12	1.85	0.57
1:B:372:ASN:OD1	1:B:443:ASP:OD2	2.22	0.57
1:A:431:LYS:HE3	1:A:432:GLU:OE1	2.05	0.57
1:A:174:LYS:HB3	1:A:175:PRO:CD	2.35	0.57
1:B:101:ILE:HD11	1:B:311:MET:CG	2.35	0.57
1:A:297:PRO:O	1:A:298:GLN:CB	2.51	0.57
1:A:65:ARG:HG3	1:A:67:VAL:CG2	2.30	0.56
1:B:164:ILE:HD12	1:B:164:ILE:N	2.19	0.56
1:B:288:ARG:HD2	1:B:321:HIS:HB2	1.87	0.56
1:A:8:VAL:HG21	1:A:39:VAL:HG13	1.85	0.56
1:B:30:MET:HA	1:B:120:TYR:O	2.05	0.56
1:A:288:ARG:NE	1:A:291:HIS:CE1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:HA	1:A:278:ARG:NE	2.15	0.56
1:A:96:ASP:OD1	1:A:277:ARG:NH1	2.37	0.56
1:A:143:ILE:O	1:A:146:LEU:HB2	2.06	0.55
1:B:447:ILE:O	1:B:449:PRO:HD3	2.05	0.55
1:A:167:PRO:HG3	1:B:53:THR:HG22	1.89	0.55
1:A:204:LEU:HD22	1:B:94:ILE:HD13	1.89	0.55
1:B:400:ILE:HG22	1:B:439:SER:OG	2.06	0.55
1:A:7:TYR:CE2	1:A:47:ALA:HB2	2.41	0.55
1:A:7:TYR:CD2	1:A:47:ALA:HB2	2.42	0.55
1:A:38:TYR:HE2	1:A:74:VAL:HG22	1.72	0.55
1:B:364:THR:HG22	1:B:365:PRO:O	2.07	0.55
1:B:447:ILE:HG13	1:B:448:TYR:CD2	2.42	0.55
1:B:241:ILE:HG12	1:B:278:ARG:CG	2.35	0.55
1:A:393:GLY:C	1:A:395:GLY:H	2.08	0.54
1:B:321:HIS:HB3	2:B:500:3PG:P	2.46	0.54
1:B:270:ALA:O	1:B:274:THR:OG1	2.18	0.54
1:B:423:VAL:HG13	1:B:433:LEU:HD21	1.89	0.54
1:A:74:VAL:HA	1:A:80:LEU:O	2.06	0.54
1:A:443:ASP:HA	1:A:446:GLN:HG3	1.89	0.54
1:B:291:HIS:O	1:B:293:ALA:N	2.41	0.54
1:A:64:THR:HG22	1:A:68:ASP:OD1	2.08	0.53
1:B:272:ILE:HG21	1:B:315:GLN:NE2	2.23	0.53
1:B:296:SER:CB	1:B:299:SER:HB2	2.37	0.53
1:A:123:MET:HE3	1:A:307:VAL:HG11	1.89	0.53
1:A:297:PRO:HG2	1:B:301:ARG:NH2	2.23	0.53
1:B:288:ARG:HB3	1:B:308:HIS:HE1	1.74	0.53
1:B:336:ASP:HA	1:B:339:ILE:HD12	1.90	0.53
1:A:168:LYS:O	1:A:196:GLN:NE2	2.40	0.53
1:A:186:GLY:HA2	1:A:408:ARG:HD2	1.90	0.53
2:A:500:3PG:O3	1:B:111:ASN:ND2	2.39	0.53
1:A:337:ARG:HE	1:A:341:TYR:HE1	1.55	0.53
1:B:412:GLN:OE1	1:B:432:GLU:HB2	2.09	0.53
1:A:296:SER:HB3	1:A:299:SER:H	1.73	0.53
1:A:424:LEU:O	1:A:428:ARG:HD3	2.09	0.53
1:B:294:VAL:HG13	1:B:302:GLY:HA3	1.91	0.53
1:B:372:ASN:HD21	1:B:374:LEU:HB2	1.74	0.53
1:B:335:SER:C	1:B:339:ILE:CD1	2.78	0.52
1:A:290:GLY:HA3	1:B:110:GLY:O	2.09	0.52
1:A:397:PHE:HE2	1:A:410:LEU:HD12	1.74	0.52
1:A:104:PHE:O	1:A:108:THR:HB	2.08	0.52
1:A:450:GLY:O	1:A:453:LYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:CG2	1:B:133:ARG:HB2	2.37	0.52
1:A:200:PRO:HD2	1:B:88:ALA:O	2.10	0.52
1:A:392:ALA:HB1	1:A:396:ALA:CB	2.37	0.52
1:A:399:HIS:CE1	1:A:435:ARG:HB3	2.45	0.52
1:A:143:ILE:HD12	1:A:364:THR:HG21	1.92	0.52
1:A:451:TRP:CZ2	1:A:452:ARG:HG3	2.45	0.51
1:A:444:ALA:O	1:A:445:ASP:C	2.49	0.51
1:B:3:GLN:NE2	1:B:44:HIS:CB	2.67	0.51
1:B:3:GLN:HE22	1:B:47:ALA:HB3	1.76	0.51
1:B:153:PRO:HD2	1:B:157:GLY:HA2	1.93	0.51
1:B:169:LEU:HD13	1:B:196:GLN:HG2	1.91	0.51
1:B:164:ILE:HD12	1:B:164:ILE:H	1.74	0.51
1:A:168:LYS:HE2	1:A:194:GLU:HG2	1.91	0.51
1:B:101:ILE:HD11	1:B:311:MET:HG3	1.92	0.51
1:A:374:LEU:HB3	1:A:448:TYR:CE2	2.45	0.51
1:A:445:ASP:O	1:A:446:GLN:C	2.48	0.51
1:B:164:ILE:HD11	1:B:391:THR:HG23	1.91	0.51
1:A:247:VAL:O	1:A:251:PHE:HD2	1.94	0.51
1:A:285:HIS:NE2	1:A:321:HIS:NE2	2.59	0.51
1:A:321:HIS:CB	2:A:500:3PG:O3P	2.58	0.51
1:B:222:THR:CG2	1:B:224:GLU:HB2	2.35	0.51
1:B:385:ASN:HB2	1:B:387:ASN:ND2	2.26	0.51
1:A:194:GLU:HG3	1:A:195:PRO:CG	2.37	0.51
1:A:296:SER:CB	1:A:297:PRO:CD	2.86	0.51
1:B:87:VAL:O	1:B:92:ARG:NH2	2.43	0.51
1:A:285:HIS:NE2	1:A:321:HIS:HD2	2.09	0.50
1:B:341:TYR:O	1:B:345:GLN:HB2	2.11	0.50
1:A:299:SER:C	1:A:301:ARG:N	2.63	0.50
1:A:344:THR:HA	1:A:362:ALA:CB	2.37	0.50
1:A:376:MET:HA	1:A:376:MET:CE	2.41	0.50
1:B:342:MET:HA	1:B:348:ALA:CB	2.41	0.50
1:A:72:TYR:CZ	1:A:82:LYS:HB3	2.46	0.50
1:A:87:VAL:HG11	1:A:132:TYR:HB2	1.93	0.50
1:A:96:ASP:HB3	1:A:98:LYS:H	1.77	0.50
1:B:30:MET:HB2	1:B:121:ALA:HB2	1.92	0.50
1:A:165:ILE:HG21	1:A:176:PHE:CE2	2.47	0.50
1:B:6:ARG:HG2	1:B:7:TYR:CE2	2.47	0.50
1:B:205:ARG:HA	1:B:246:TYR:CE1	2.47	0.50
1:B:261:LEU:CD1	1:B:287:HIS:HB2	2.41	0.50
1:A:183:PHE:CE1	1:A:187:GLY:HA3	2.47	0.50
1:A:88:ALA:O	1:B:200:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HB3	1:B:175:PRO:CD	2.39	0.50
1:B:443:ASP:O	1:B:447:ILE:N	2.39	0.49
1:A:306:PHE:HA	1:A:339:ILE:HG12	1.94	0.49
1:A:141:VAL:HG13	1:A:145:ALA:CB	2.42	0.49
1:A:235:ASP:OD2	1:B:101:ILE:HG22	2.12	0.49
1:A:30:MET:HG2	1:A:31:LYS:N	2.27	0.49
1:A:169:LEU:HD11	1:A:195:PRO:HB2	1.93	0.49
1:B:6:ARG:HG2	1:B:7:TYR:CD2	2.46	0.49
1:A:433:LEU:O	1:A:436:ALA:HB3	2.12	0.49
1:B:261:LEU:HD11	1:B:287:HIS:HB2	1.93	0.49
1:A:50:SER:OG	1:A:69:ALA:CB	2.61	0.49
1:B:265:TYR:CE1	1:B:291:HIS:HA	2.48	0.49
1:A:382:ASN:C	1:A:382:ASN:ND2	2.65	0.49
1:A:437:PHE:HB3	1:A:451:TRP:CE3	2.48	0.49
1:A:119:GLU:O	1:A:301:ARG:NH2	2.46	0.49
1:A:261:LEU:HA	1:A:285:HIS:O	2.12	0.49
1:B:142:ASN:OD1	1:B:142:ASN:C	2.51	0.49
1:A:262:VAL:CG1	1:A:272:ILE:HD13	2.43	0.49
1:B:247:VAL:O	1:B:251:PHE:CD1	2.65	0.49
1:A:6:ARG:HE	1:A:64:THR:CG2	2.25	0.48
1:A:416:ALA:HB2	1:A:426:TYR:CG	2.48	0.48
1:B:116:GLY:O	1:B:117:ASP:CB	2.60	0.48
1:A:8:VAL:HA	1:A:71:VAL:HB	1.93	0.48
1:A:452:ARG:O	1:A:455:LEU:HA	2.13	0.48
1:A:159:LEU:HD21	1:A:161:VAL:HG23	1.95	0.48
1:B:243:ARG:O	1:B:247:VAL:HG23	2.13	0.48
1:B:324:THR:HG23	1:B:325:MET:N	2.26	0.48
1:A:70:LEU:H	1:A:70:LEU:CD1	2.26	0.48
1:A:167:PRO:CG	1:B:53:THR:HG22	2.44	0.48
1:A:111:ASN:HB2	1:B:289:ALA:HA	1.96	0.48
1:B:336:ASP:O	1:B:337:ARG:C	2.49	0.48
1:B:447:ILE:HG13	1:B:448:TYR:CE2	2.49	0.48
1:A:29:ILE:HD12	1:A:80:LEU:HD12	1.95	0.48
1:A:96:ASP:OD1	1:A:277:ARG:NH2	2.44	0.48
1:A:299:SER:O	1:A:301:ARG:N	2.46	0.48
1:B:307:VAL:O	1:B:311:MET:HB2	2.14	0.48
1:B:185:LEU:O	1:B:408:ARG:NH2	2.47	0.48
1:B:292:GLY:HA2	1:B:295:THR:HG22	1.96	0.48
1:B:371:MET:SD	1:B:376:MET:HE2	2.54	0.48
1:A:447:ILE:HB	1:A:448:TYR:CD2	2.49	0.47
1:B:376:MET:HE2	1:B:376:MET:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ALA:O	1:B:222:THR:HB	2.15	0.47
1:A:222:THR:CG2	1:A:224:GLU:H	2.27	0.47
1:A:297:PRO:O	1:A:298:GLN:HB2	2.13	0.47
1:B:8:VAL:HG23	1:B:43:ALA:HB2	1.97	0.47
1:B:50:SER:HB3	1:B:69:ALA:CB	2.45	0.47
1:A:96:ASP:CB	1:A:98:LYS:HB2	2.43	0.47
1:A:65:ARG:O	1:A:65:ARG:CD	2.62	0.47
1:A:296:SER:C	1:A:298:GLN:N	2.67	0.47
1:A:183:PHE:HE2	1:A:397:PHE:CE1	2.33	0.47
1:A:6:ARG:HH21	1:A:64:THR:HG23	1.80	0.46
1:A:38:TYR:CE2	1:A:74:VAL:HG13	2.51	0.46
1:B:30:MET:HB2	1:B:121:ALA:CB	2.45	0.46
1:B:400:ILE:HG12	1:B:400:ILE:O	2.15	0.46
1:A:236:ASP:O	1:A:239:GLU:HB3	2.15	0.46
1:B:166:LYS:HG2	1:B:167:PRO:HA	1.97	0.46
1:A:130:GLU:O	1:A:130:GLU:HG2	2.14	0.46
1:A:205:ARG:HA	1:A:246:TYR:CE2	2.50	0.46
1:B:344:THR:HA	1:B:362:ALA:HB1	1.97	0.46
1:B:372:ASN:ND2	1:B:374:LEU:H	2.06	0.46
1:B:411:ARG:O	1:B:414:TRP:HB3	2.16	0.46
1:A:16:ASP:O	1:A:20:GLY:N	2.49	0.46
1:A:94:ILE:HD12	1:B:205:ARG:NH1	2.31	0.46
1:A:371:MET:HB2	1:A:376:MET:HE3	1.96	0.46
1:A:431:LYS:HB2	1:A:432:GLU:OE1	2.15	0.46
1:A:6:ARG:NH2	1:A:64:THR:HG23	2.31	0.46
1:A:289:ALA:O	1:B:111:ASN:HA	2.14	0.46
1:B:81:THR:HG22	1:B:83:ILE:HD11	1.98	0.46
1:B:254:ASN:O	1:B:257:HIS:HB2	2.16	0.46
1:A:18:ILE:HG23	1:A:127:TYR:CZ	2.50	0.46
1:A:427:ALA:O	1:A:434:ALA:HB2	2.16	0.45
1:B:50:SER:HB3	1:B:69:ALA:HB2	1.98	0.45
1:B:400:ILE:HD13	1:B:435:ARG:NH2	2.31	0.45
1:A:25:LEU:HD12	1:A:84:ALA:HB2	1.98	0.45
1:A:109:MET:CE	1:A:123:MET:HE1	2.47	0.45
1:A:239:GLU:O	1:A:243:ARG:HG3	2.15	0.45
1:A:75:ASP:OD1	1:A:78:ARG:NH1	2.49	0.45
1:B:276:ARG:HB2	1:B:284:LEU:CD1	2.46	0.45
1:A:295:THR:HG23	1:A:305:ALA:CA	2.46	0.45
1:B:169:LEU:HD11	1:B:196:GLN:HA	1.97	0.45
1:B:174:LYS:CB	1:B:175:PRO:CD	2.94	0.45
1:A:113:GLN:OE1	1:A:121:ALA:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:HA	1:A:455:LEU:HD12	1.75	0.45
1:B:7:TYR:O	1:B:70:LEU:HA	2.16	0.45
1:B:448:TYR:O	1:B:451:TRP:HB3	2.16	0.45
1:A:294:VAL:CG1	1:A:295:THR:N	2.78	0.45
1:B:272:ILE:HG21	1:B:315:GLN:HE21	1.82	0.45
1:B:168:LYS:HG2	1:B:169:LEU:HD22	1.99	0.45
1:B:209:ALA:HA	1:B:250:THR:HG21	1.99	0.45
1:B:276:ARG:HB2	1:B:284:LEU:HD12	1.99	0.45
1:B:444:ALA:O	1:B:445:ASP:C	2.55	0.45
1:B:162:GLY:CA	1:B:189:PHE:O	2.61	0.44
1:A:291:HIS:H	1:A:291:HIS:HD2	1.47	0.44
1:A:431:LYS:H	1:A:431:LYS:HG3	1.39	0.44
1:A:38:TYR:HE2	1:A:74:VAL:CG2	2.30	0.44
1:A:243:ARG:O	1:A:244:GLY:C	2.55	0.44
1:A:295:THR:CG2	1:A:305:ALA:HB2	2.46	0.44
1:A:337:ARG:NE	1:A:341:TYR:HE1	2.15	0.44
1:A:367:ILE:HG22	1:A:390:LEU:HD12	1.98	0.44
1:A:437:PHE:HB3	1:A:451:TRP:CZ3	2.52	0.44
1:B:343:LEU:HB3	1:B:363:CYS:O	2.17	0.44
1:A:191:LYS:HE2	1:A:192:ASN:O	2.18	0.44
1:A:101:ILE:HD12	1:A:101:ILE:HA	1.97	0.44
1:A:104:PHE:CE2	1:A:109:MET:HE2	2.52	0.44
1:B:101:ILE:HD11	1:B:311:MET:HG2	1.98	0.44
1:B:231:ASN:HD21	1:B:233:THR:HB	1.82	0.44
1:A:294:VAL:HG12	1:A:295:THR:H	1.81	0.44
1:A:51:THR:HG22	1:B:169:LEU:O	2.18	0.43
1:A:128:VAL:HA	1:A:129:PRO:HD3	1.71	0.43
1:A:208:ILE:HG21	1:A:247:VAL:HG22	2.00	0.43
1:A:421:VAL:CG1	1:A:426:TYR:HB2	2.48	0.43
1:A:76:GLU:H	1:A:76:GLU:HG2	1.59	0.43
1:B:273:THR:HG22	1:B:273:THR:O	2.18	0.43
1:B:322:THR:HG21	1:B:365:PRO:HB3	2.01	0.43
1:B:376:MET:CB	1:B:377:PRO:CD	2.89	0.43
1:B:165:ILE:HD13	1:B:165:ILE:HA	1.94	0.43
1:B:444:ALA:O	1:B:448:TYR:N	2.50	0.43
1:A:80:LEU:HD21	1:A:82:LYS:HE3	2.01	0.43
1:A:172:ARG:HB3	1:A:173:PRO:HD2	2.00	0.43
1:B:93:ASN:ND2	1:B:96:ASP:HB2	2.16	0.43
1:B:138:GLY:HA2	1:B:313:ARG:O	2.18	0.43
1:B:336:ASP:HA	1:B:339:ILE:CB	2.47	0.43
1:A:98:LYS:HG3	1:A:135:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HD2	1:A:285:HIS:HE1	1.82	0.43
1:B:436:ALA:O	1:B:439:SER:N	2.51	0.43
1:A:65:ARG:O	1:A:65:ARG:CG	2.66	0.43
1:A:163:THR:HG23	1:A:397:PHE:CD1	2.52	0.43
1:B:120:TYR:HB2	1:B:300:LYS:O	2.18	0.43
1:A:288:ARG:NE	1:A:291:HIS:HE1	2.17	0.43
1:A:101:ILE:HD11	1:A:311:MET:HG2	2.01	0.42
1:B:296:SER:HA	1:B:297:PRO:HD3	1.62	0.42
1:A:222:THR:HG23	1:A:224:GLU:HG3	2.01	0.42
1:A:337:ARG:HD2	1:A:382:ASN:HD21	1.84	0.42
1:B:159:LEU:HD12	1:B:160:VAL:N	2.34	0.42
1:A:168:LYS:HB2	1:A:193:ASP:OD1	2.19	0.42
1:A:337:ARG:O	1:A:337:ARG:HG2	2.18	0.42
1:B:379:PHE:O	1:B:383:LEU:HB3	2.19	0.42
2:A:500:3PG:O3	1:B:111:ASN:OD1	2.34	0.42
1:B:184:TRP:CG	1:B:226:LYS:HD3	2.55	0.42
1:A:150:LEU:CG	1:A:227:LEU:HD11	2.48	0.42
1:B:374:LEU:HD22	1:B:448:TYR:CD2	2.55	0.42
1:B:451:TRP:O	1:B:455:LEU:HB2	2.19	0.42
1:A:8:VAL:HG21	1:A:39:VAL:CG1	2.50	0.42
1:A:123:MET:CE	1:A:307:VAL:HG11	2.50	0.42
1:A:402:GLY:O	1:A:406:GLY:N	2.52	0.42
1:B:261:LEU:HD11	1:B:287:HIS:CB	2.50	0.42
1:B:273:THR:O	1:B:277:ARG:HG3	2.19	0.42
1:A:50:SER:HB3	1:A:51:THR:H	1.59	0.42
1:B:367:ILE:HG12	1:B:379:PHE:HZ	1.85	0.42
1:A:152:ARG:HB3	1:A:153:PRO:CD	2.48	0.42
1:B:372:ASN:OD1	1:B:375:ARG:NH1	2.52	0.42
1:B:103:SER:O	1:B:107:LEU:HB2	2.20	0.41
1:B:168:LYS:HG3	1:B:193:ASP:OD2	2.19	0.41
1:B:372:ASN:O	1:B:376:MET:HE3	2.20	0.41
1:B:424:LEU:HD23	1:B:454:ALA:CB	2.50	0.41
1:A:399:HIS:HE1	1:A:435:ARG:HB3	1.85	0.41
1:B:3:GLN:HE21	1:B:44:HIS:CG	2.38	0.41
1:B:334:SER:O	1:B:338:ALA:HB3	2.20	0.41
1:A:300:LYS:H	1:A:300:LYS:HG2	1.48	0.41
1:B:41:THR:HG22	1:B:118:VAL:HG22	2.03	0.41
1:B:291:HIS:NE2	1:B:295:THR:HG21	2.34	0.41
1:A:191:LYS:HD2	1:A:285:HIS:CE1	2.55	0.41
1:B:433:LEU:HD12	1:B:433:LEU:HA	1.97	0.41
1:B:24:VAL:HG21	1:B:90:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD22	1:A:127:TYR:HD1	1.86	0.41
1:A:31:LYS:HA	1:A:32:PRO:HD3	1.88	0.41
1:A:126:PHE:CD1	1:A:307:VAL:HG13	2.56	0.41
1:A:319:GLY:HA2	1:A:364:THR:O	2.20	0.41
1:B:152:ARG:HB3	1:B:153:PRO:CD	2.51	0.41
1:B:336:ASP:HA	1:B:339:ILE:CG1	2.51	0.41
1:B:456:GLY:O	1:B:457:VAL:CB	2.63	0.41
1:A:31:LYS:O	1:A:119:GLU:HB2	2.20	0.41
1:A:143:ILE:HB	1:A:364:THR:OG1	2.20	0.41
1:A:148:LYS:HB2	1:A:154:GLU:HG2	2.03	0.41
1:A:261:LEU:HD11	1:A:287:HIS:HB2	2.02	0.41
1:B:244:GLY:HA3	1:B:279:PHE:CZ	2.56	0.41
1:A:139:PRO:HD3	1:A:313:ARG:O	2.21	0.40
1:B:45:PHE:CA	1:B:115:MET:HE3	2.43	0.40
1:B:159:LEU:HD12	1:B:160:VAL:H	1.86	0.40
1:B:184:TRP:HB3	1:B:226:LYS:HD3	2.03	0.40
1:A:336:ASP:HA	1:A:339:ILE:HD12	2.02	0.40
1:A:337:ARG:NE	1:A:341:TYR:CE1	2.88	0.40
1:A:434:ALA:O	1:A:437:PHE:HB2	2.21	0.40
1:B:33:LYS:O	1:B:34:ALA:C	2.60	0.40
1:B:41:THR:HG23	1:B:117:ASP:O	2.21	0.40
1:B:286:TYR:HB2	1:B:317:ALA:HB1	2.04	0.40
1:A:30:MET:HE1	1:A:32:PRO:HG3	2.03	0.40
1:A:146:LEU:HD22	1:A:227:LEU:HD22	2.03	0.40
1:A:165:ILE:HD11	1:A:190:ILE:HG21	2.02	0.40
1:A:307:VAL:O	1:A:311:MET:HB2	2.22	0.40
1:B:168:LYS:HG3	1:B:193:ASP:CG	2.42	0.40
1:B:265:TYR:CZ	1:B:291:HIS:HA	2.56	0.40
1:B:366:ILE:HD13	1:B:366:ILE:HG21	1.85	0.40
1:A:278:ARG:HE	1:A:278:ARG:CA	2.09	0.40
1:B:172:ARG:HE	1:B:172:ARG:HB3	1.61	0.40

All (2) 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)
1:A:346:ASP:OD2	1:A:408:ARG:NH2[2_646]	1.89	0.31
1:A:358:GLY:O	1:A:431:LYS:CD[2_646]	2.07	0.13

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%)	374 (87%)	38 (9%)	19 (4%)	2	10
1	B	429/490 (88%)	365 (85%)	46 (11%)	18 (4%)	3	10
All	All	860/980 (88%)	739 (86%)	84 (10%)	37 (4%)	2	10

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	298	GLN
1	A	372	ASN
1	B	4	SER
1	B	5	SER
1	B	34	ALA
1	B	50	SER
1	B	110	GLY
1	B	291	HIS
1	B	292	GLY
1	A	252	GLY
1	A	335	SER
1	A	431	LYS
1	A	455	LEU
1	B	117	ASP
1	B	335	SER
1	B	423	VAL
1	A	300	LYS
1	A	446	GLN
1	B	49	SER
1	B	184	TRP
1	A	10	LEU
1	A	34	ALA
1	A	115	MET
1	A	119	GLU

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Mol	Chain	Res	Type
1	A	184	TRP
1	A	290	GLY
1	A	297	PRO
1	B	9	ASN
1	B	195	PRO
1	A	444	ALA
1	A	456	GLY
1	B	79	GLU
1	B	393	GLY
1	B	129	PRO
1	B	194	GLU
1	A	296	SER

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%)	254 (77%)	76 (23%)	1	2
1	B	327/376 (87%)	276 (84%)	51 (16%)	2	8
All	All	657/752 (87%)	530 (81%)	127 (19%)	1	4

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ARG
1	A	8	VAL
1	A	22	GLU
1	A	25	LEU
1	A	29	ILE
1	A	30	MET
1	A	31	LYS
1	A	33	LYS
1	A	45	PHE
1	A	50	SER

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Mol	Chain	Res	Type
1	A	64	THR
1	A	65	ARG
1	A	70	LEU
1	A	74	VAL
1	A	76	GLU
1	A	92	ARG
1	A	98	LYS
1	A	105	LEU
1	A	106	THR
1	A	107	LEU
1	A	109	MET
1	A	113	GLN
1	A	117	ASP
1	A	119	GLU
1	A	122	LYS
1	A	141	VAL
1	A	161	VAL
1	A	163	THR
1	A	168	LYS
1	A	171	LEU
1	A	174	LYS
1	A	191	LYS
1	A	192	ASN
1	A	196	GLN
1	A	204	LEU
1	A	210	LEU
1	A	222	THR
1	A	226	LYS
1	A	231	ASN
1	A	266	VAL
1	A	272	ILE
1	A	278	ARG
1	A	284	LEU
1	A	286	TYR
1	A	288	ARG
1	A	291	HIS
1	A	294	VAL
1	A	296	SER
1	A	298	GLN
1	A	300	LYS
1	A	301	ARG
1	A	308	HIS

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Mol	Chain	Res	Type
1	A	311	MET
1	A	322	THR
1	A	324	THR
1	A	325	MET
1	A	334	SER
1	A	336	ASP
1	A	337	ARG
1	A	344	THR
1	A	356	SER
1	A	371	MET
1	A	375	ARG
1	A	376	MET
1	A	382	ASN
1	A	385	ASN
1	A	408	ARG
1	A	428	ARG
1	A	431	LYS
1	A	432	GLU
1	A	435	ARG
1	A	443	ASP
1	A	445	ASP
1	A	446	GLN
1	A	448	TYR
1	B	9	ASN
1	B	10	LEU
1	B	30	MET
1	B	73	GLU
1	B	106	THR
1	B	107	LEU
1	B	111	ASN
1	B	112	ASN
1	B	113	GLN
1	B	115	MET
1	B	117	ASP
1	B	119	GLU
1	B	141	VAL
1	B	163	THR
1	B	169	LEU
1	B	172	ARG
1	B	174	LYS
1	B	178	GLU
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	201	PHE
1	B	205	ARG
1	B	222	THR
1	B	226	LYS
1	B	227	LEU
1	B	261	LEU
1	B	266	VAL
1	B	286	TYR
1	B	287	HIS
1	B	288	ARG
1	B	295	THR
1	B	301	ARG
1	B	324	THR
1	B	325	MET
1	B	337	ARG
1	B	345	GLN
1	B	354	ARG
1	B	367	ILE
1	B	371	MET
1	B	376	MET
1	B	382	ASN
1	B	391	THR
1	B	400	ILE
1	B	422	PRO
1	B	424	LEU
1	B	425	ASP
1	B	431	LYS
1	B	443	ASP
1	B	446	GLN
1	B	447	ILE
1	B	452	ARG
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	291	HIS
1	A	321	HIS
1	A	382	ASN
1	A	385	ASN
1	A	415	GLN

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Mol	Chain	Res	Type
1	B	9	ASN
1	B	93	ASN
1	B	231	ASN
1	B	315	GLN
1	B	372	ASN
1	B	415	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3PG	B	500	-	9,10,10	1.90	3 (33%)	12,14,14	2.24	3 (25%)
2	3PG	A	500	-	9,10,10	3.61	6 (66%)	12,14,14	3.66	10 (83%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3PG	B	500	-	-	6/10/10/10	-
2	3PG	A	500	-	-	7/10/10/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	3PG	P-O1P	8.17	1.86	1.60
2	A	500	3PG	O1P-C3	3.78	1.59	1.44
2	A	500	3PG	P-O2P	3.72	1.62	1.50
2	B	500	3PG	P-O2P	3.32	1.61	1.50
2	A	500	3PG	O1-C1	2.87	1.30	1.22
2	B	500	3PG	O1-C1	2.59	1.30	1.22
2	A	500	3PG	P-O4P	2.56	1.64	1.54
2	A	500	3PG	P-O3P	2.18	1.63	1.54
2	B	500	3PG	O1P-C3	-2.07	1.36	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	3PG	P-O1P-C3	5.82	134.32	118.30
2	A	500	3PG	O2-C1-C2	5.47	124.74	112.72
2	B	500	3PG	O1P-C3-C2	5.15	122.81	107.94
2	A	500	3PG	O1P-C3-C2	4.65	121.36	107.94
2	A	500	3PG	O3-C2-C1	-3.93	99.88	110.36
2	A	500	3PG	O1P-P-O2P	3.91	117.44	106.47
2	A	500	3PG	O3P-P-O1P	3.59	116.29	106.73
2	B	500	3PG	O2-C1-C2	3.42	120.23	112.72
2	A	500	3PG	O2-C1-O1	-2.72	117.90	124.09
2	A	500	3PG	O1-C1-C2	-2.67	117.32	122.54
2	A	500	3PG	O4P-P-O1P	2.56	113.55	106.73
2	B	500	3PG	O2-C1-O1	-2.35	118.75	124.09
2	A	500	3PG	O4P-P-O2P	-2.32	101.61	110.68

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	3PG	O1-C1-C2-O3
2	A	500	3PG	O2-C1-C2-O3
2	A	500	3PG	C1-C2-C3-O1P
2	A	500	3PG	O3-C2-C3-O1P
2	B	500	3PG	C2-C3-O1P-P

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Mol	Chain	Res	Type	Atoms
2	B	500	3PG	C3-O1P-P-O2P
2	B	500	3PG	C3-O1P-P-O3P
2	B	500	3PG	C3-O1P-P-O4P
2	A	500	3PG	O1-C1-C2-C3
2	A	500	3PG	O2-C1-C2-C3
2	B	500	3PG	O1-C1-C2-C3
2	B	500	3PG	O2-C1-C2-O3
2	A	500	3PG	C2-C3-O1P-P

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	3PG	5	0
2	A	500	3PG	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.