Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:02 PM GMT

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.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

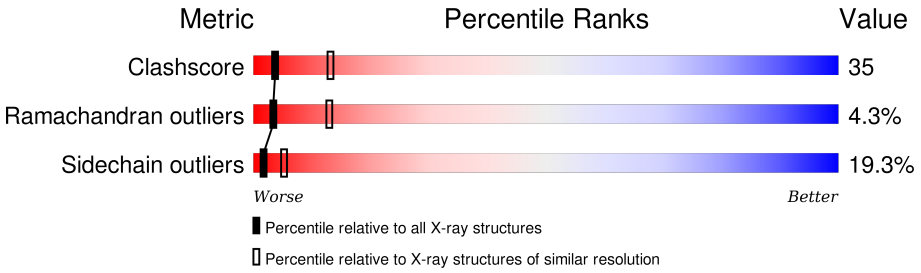
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	490	32% 33% 17% 7% 11%
1	B	490	33% 36% 17% • 11%

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	-
2	3PG	B	500	-	-	X	-

2 Entry composition

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.

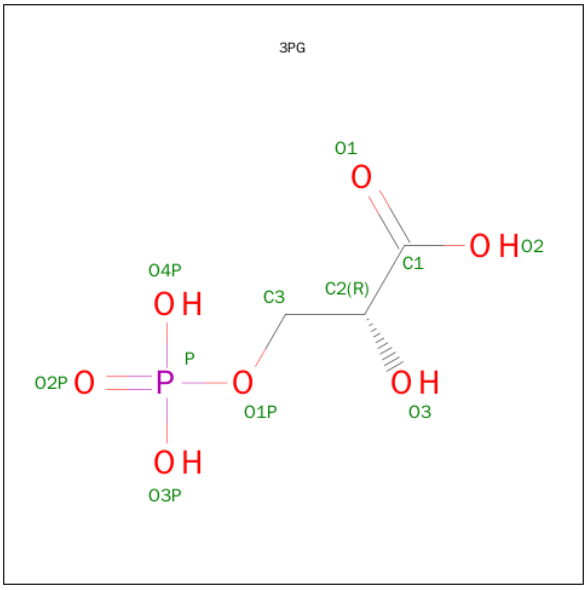
- Molecule 1 is a protein called RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	7	0	0
			3337	2115	589	617	16			
1	B	435	Total	C	N	O	S	10	0	0
			3318	2105	584	613	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 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: $C_3H_7O_7P$).



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

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

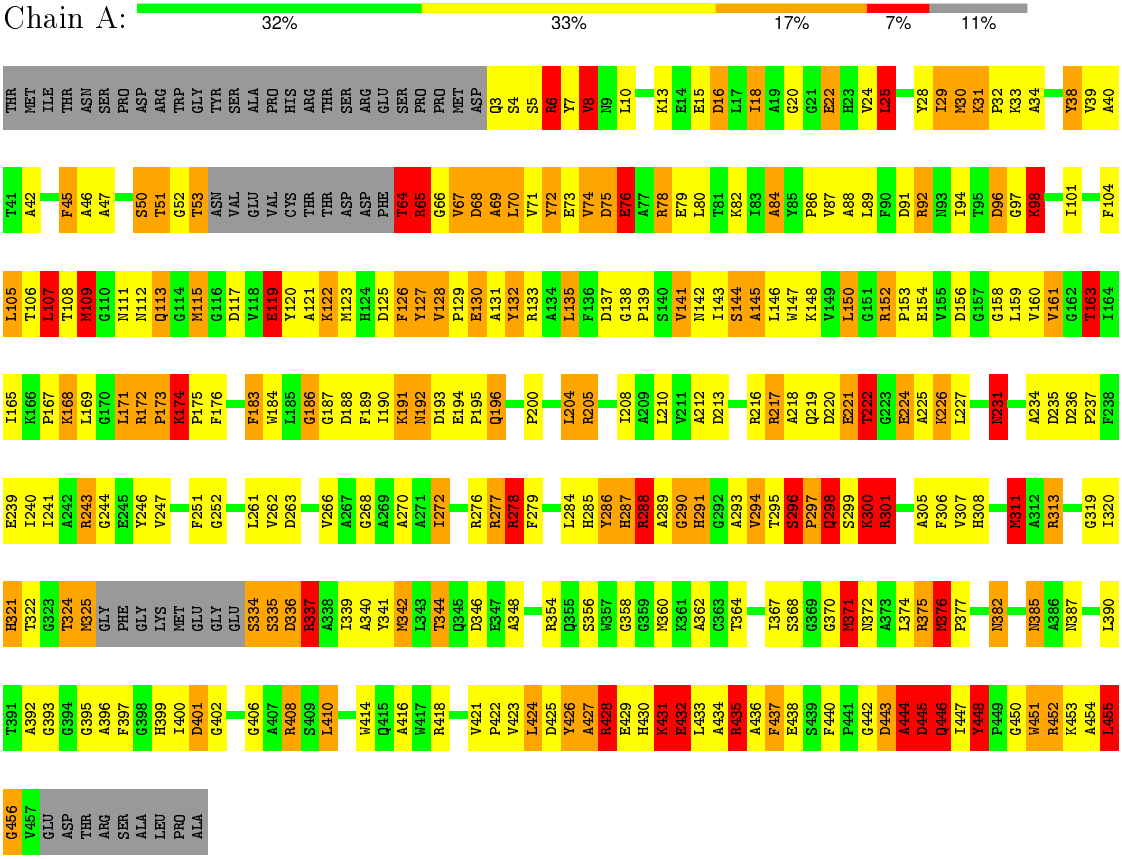
3 Residue-property plots (i)

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

Note EDS was not executed.

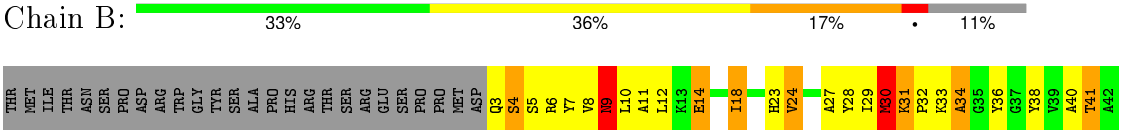
• Molecule 1: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)

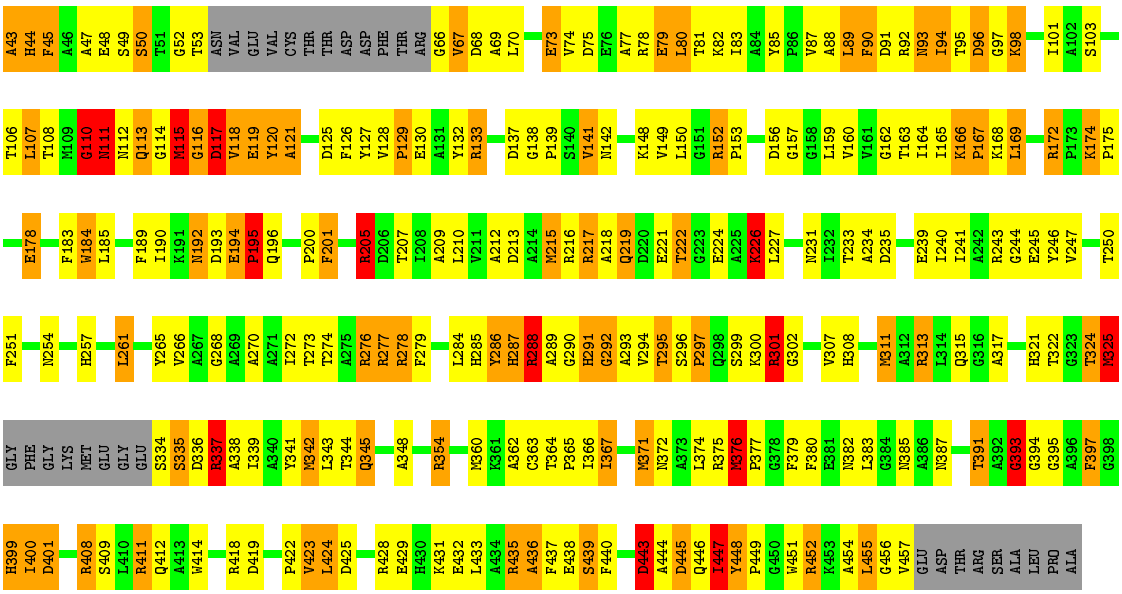
Chain A:



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

Chain B:




A43 H44 F45 A46 A47 E48 S49 S50 T51 G52 T53 ASN VAL GLU VAL CYS THR THR ASP ASP PHE THR ARG G66 V67 D68 A69 L70 E73 V74 D75 E76 A77 R78 E79 L80 T81 K82 I83 A84 Y85 F86 V87 A88 L89 F90 D91 R92 N93 I94 T95 D96 G97 K98 I101 A102 S103
T106 L107 T108 M109 G110 N111 N112 Q113 G114 M115 G116 D117 V118 E119 Y120 A121 D125 F126 Y127 V128 P129 E130 A131 Y132 R133 D137 G138 P139 S140 V141 N142 K148 V149 L150 G151 R152 P153 D156 G157 G158 L159 V160 V161 G162 T163 I164 I165 K166 P167 K168 L169 R172 P173 K174 P175
E178 F183 W184 L185 F189 I190 K191 N192 D193 E194 P195 Q196 P200 F201 R205 D206 T207 I208 A209 L210 V211 A212 D213 A214 M215 R216 R217 A218 Q219 D220 E221 T222 G223 E224 A225 K226 L227 N231 I232 T233 A234 D235 E239 I240 I241 A242 R243 G244 E245 Y246 V247 T250
F251 N254 H257 L261 Y265 V266 A267 G268 A269 A270 A271 I272 T273 T274 A275 R276 R277 R278 F279 L284 H285 Y286 H287 R288 A289 G290 H291 G292 A293 V294 T295 S296 P297 Q298 S299 K300 R301 G302 V307 H308 M311 A312 R313 L314 Q315 G316 A317 H321 T322 G323 T324 M325
GLY PHE GLY LYS MET GLU GLY GLU S334 S335 D336 R337 A338 I339 A340 Y341 M342 L343 T344 Q345 A348 R354 M360 K361 A362 C363 T364 P365 I366 I367 M371 N372 A373 L374 R375 N376 P377 G378 F379 F380 E381 N382 L383 G384 N385 A386 N387 T391 A392 G393 G394 G395 A396 F397 G398
H399 I400 D401 R408 S409 L410 R411 Q412 A413 W414 R418 D419 P422 V423 L424 D425 R428 E429 H430 K431 E432 L433 A434 R435 A436 F437 E438 S439 F440 D443 A444 D445 Q446 T447 Y448 P449 G450 W451 R452 K453 A454 L455 G456 V457 GLU ASP THR ARG SER ALA LEU PRO ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 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

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:335:SER:C	1:B:339:ILE:HG13	1.74	1.06
1:B:324:THR:HG22	1:B:325:MET:H	1.19	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:HA	1:A:278:ARG:HE	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:B:74:VAL:HA	1:B:80:LEU:O	1.87	0.73
1:A:167:PRO:HB3	1:B:53:THR:HG22	1.69	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:370:GLY:HA3	1:A:396:ALA:HB2	1.72	0.71
1:A:107:LEU:HD13	1:B:195:PRO:HB3	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:B:290:GLY:O	1:B:292:GLY:N	2.23	0.71
1:A:400:ILE:HD11	1:A:435:ARG:HG3	1.71	0.71
1:B:321:HIS:ND1	2:B:500:3PG:O4P	2.23	0.71
1:A:174:LYS:HB3	1:A:175:PRO:HD3	1.72	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:285:HIS:HE2	1:B:321:HIS:CD2	2.10	0.69
1:B:192:ASN:ND2	1:B:196:GLN:OE1	2.24	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:B:301:ARG:HH11	1:B:301:ARG:HG2	1.59	0.68
1:A:431:LYS:O	1:A:434:ALA:HB3	1.94	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:B:321:HIS:CG	2:B:500:3PG:O4P	2.48	0.66
1:A:342:MET:HA	1:A:348:ALA:CB	2.26	0.66
1:B:278:ARG:O	1:B:278:ARG:HD3	1.94	0.66
1:A:370:GLY:CA	1:A:396:ALA:HB2	2.25	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:O	1:A:65:ARG:HD2	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:B:335:SER:C	1:B:339:ILE:CG1	2.54	0.64
1:A:217:ARG:O	1:A:221:GLU:HG3	1.97	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:B:3:GLN:HE22	1:B:44:HIS:HA	1.59	0.61
1:A:278:ARG:HG3	1:A:279:PHE:CD1	2.34	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:424:LEU:HD13	1:A:437:PHE:CZ	2.34	0.61
1:A:150:LEU:HG	1:A:227:LEU:HD11	1.83	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:N	1:A:70:LEU:HD12	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:O	1:B:447:ILE:HD12	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:168:LYS:HE2	1:B:193:ASP:OD2	2.02	0.59
1:B:129:PRO:HG2	1:B:132:TYR:HB3	1.83	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:B:457:VAL:HG12	1:B:457:VAL:O	2.02	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: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:424:LEU:HD11	1:B:448:TYR:HB3	1.86	0.57
1:B:393:GLY:O	1:B:397:PHE:HB2	2.03	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:B:288:ARG:HD2	1:B:321:HIS:HB2	1.87	0.56
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:30:MET:HA	1:B:120:TYR:O	2.05	0.56
1:A:8:VAL:HG21	1:A:39:VAL:HG13	1.85	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:B:447:ILE:O	1:B:449:PRO:HD3	2.05	0.55
1:A:143:ILE:O	1:A:146:LEU:HB2	2.06	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:38:TYR:HE2	1:A:74:VAL:HG22	1.72	0.55
1:A:7:TYR:CD2	1:A:47:ALA:HB2	2.42	0.55
1:A:7:TYR:CE2	1:A:47:ALA:HB2	2.41	0.55
1:B:447:ILE:HG13	1:B:448:TYR:CD2	2.42	0.55
1:B:364:THR:HG22	1:B:365:PRO:O	2.07	0.55
1:B:241:ILE:HG12	1:B:278:ARG:CG	2.35	0.55
1:B:321:HIS:HB3	2:B:500:3PG:P	2.46	0.54
1:A:393:GLY:C	1:A:395:GLY:H	2.08	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:443:ASP:HA	1:A:446:GLN:HG3	1.89	0.54
1:A:74:VAL:HA	1:A:80:LEU:O	2.06	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:296:SER:CB	1:B:299:SER:HB2	2.37	0.53
1:B:272:ILE:HG21	1:B:315:GLN:NE2	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:297:PRO:HG2	1:B:301:ARG:NH2	2.23	0.53
1:A:123:MET:HE3	1:A:307:VAL:HG11	1.89	0.53
1:A:168:LYS:O	1:A:196:GLN:NE2	2.40	0.53
2:A:500:3PG:O3	1:B:111:ASN:ND2	2.39	0.53
1:A:186:GLY:HA2	1:A:408:ARG:HD2	1.90	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:B:372:ASN:HD21	1:B:374:LEU:HB2	1.74	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:335:SER:C	1:B:339:ILE:CD1	2.78	0.52
1:A:397:PHE:HE2	1:A:410:LEU:HD12	1.74	0.52
1:A:290:GLY:HA3	1:B:110:GLY:O	2.09	0.52
1:B:128:VAL:CG2	1:B:133:ARG:HB2	2.37	0.52
1:A:104:PHE:O	1:A:108:THR:HB	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:GLY:O	1:A:453:LYS:HB3	2.09	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:200:PRO:HD2	1:B:88:ALA:O	2.10	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: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:169:LEU:HD13	1:B:196:GLN:HG2	1.91	0.51
1:A:444:ALA:O	1:A:445:ASP:C	2.49	0.51
1:B:153:PRO:HD2	1:B:157:GLY:HA2	1.93	0.51
1:B:164:ILE:H	1:B:164:ILE:HD12	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: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:A:247:VAL:O	1:A:251:PHE:HD2	1.94	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:B:30:MET:HB2	1:B:121:ALA:HB2	1.92	0.50
1:A:96:ASP:HB3	1:A:98:LYS:H	1.77	0.50
1:B:6:ARG:HG2	1:B:7:TYR:CE2	2.47	0.50
1:A:165:ILE:HG21	1:A:176:PHE:CE2	2.47	0.50
1:B:261:LEU:CD1	1:B:287:HIS:HB2	2.41	0.50
1:B:205:ARG:HA	1:B:246:TYR:CE1	2.47	0.50
1:A:183:PHE:CE1	1:A:187:GLY:HA3	2.47	0.50
1:B:174:LYS:HB3	1:B:175:PRO:CD	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:O	1:B:200:PRO:HD2	2.12	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:235:ASP:OD2	1:B:101:ILE:HG22	2.12	0.49
1:A:141:VAL:HG13	1:A:145:ALA:CB	2.42	0.49
1:A:169:LEU:HD11	1:A:195:PRO:HB2	1.93	0.49
1:A:30:MET:HG2	1:A:31:LYS:N	2.27	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:B:265:TYR:CE1	1:B:291:HIS:HA	2.48	0.49
1:A:50:SER:OG	1:A:69:ALA:CB	2.61	0.49
1:A:437:PHE:HB3	1:A:451:TRP:CE3	2.48	0.49
1:A:382:ASN:C	1:A:382:ASN:ND2	2.65	0.49
1:A:261:LEU:HA	1:A:285:HIS:O	2.12	0.49
1:A:119:GLU:O	1:A:301:ARG:NH2	2.46	0.49
1:B:142:ASN:C	1:B:142:ASN:OD1	2.51	0.49
1:B:247:VAL:O	1:B:251:PHE:CD1	2.65	0.49
1:A:262:VAL:CG1	1:A:272:ILE:HD13	2.43	0.49
1:B:116:GLY:O	1:B:117:ASP:CB	2.60	0.48
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:A:452:ARG:O	1:A:455:LEU:HA	2.13	0.48
1:A:8:VAL:HA	1:A:71:VAL:HB	1.93	0.48
1:B:324:THR:HG23	1:B:325:MET:N	2.26	0.48
1:B:243:ARG:O	1:B:247:VAL:HG23	2.13	0.48
1:A:159:LEU:HD21	1:A:161:VAL:HG23	1.95	0.48
1:A:167:PRO:CG	1:B:53:THR:HG22	2.44	0.48
1:A:70:LEU:CD1	1:A:70:LEU:H	2.26	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:111:ASN:HB2	1:B:289:ALA:HA	1.96	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:A:96:ASP:OD1	1:A:277:ARG:NH2	2.44	0.48
1:A:29:ILE:HD12	1:A:80:LEU:HD12	1.95	0.48
1:B:292:GLY:HA2	1:B:295:THR:HG22	1.96	0.48
1:B:185:LEU:O	1:B:408:ARG:NH2	2.47	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:297:PRO:O	1:A:298:GLN:HB2	2.13	0.47
1:A:222:THR:CG2	1:A:224:GLU:H	2.27	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:296:SER:C	1:A:298:GLN:N	2.67	0.47
1:A:65:ARG:CD	1:A:65:ARG:O	2.62	0.47
1:A:183:PHE:HE2	1:A:397:PHE:CE1	2.33	0.47
1:B:30:MET:HB2	1:B:121:ALA:CB	2.45	0.46
1:B:400:ILE:O	1:B:400:ILE:HG12	2.15	0.46
1:A:38:TYR:CE2	1:A:74:VAL:HG13	2.51	0.46
1:A:6:ARG:HH21	1:A:64:THR:HG23	1.80	0.46
1:B:166:LYS:HG2	1:B:167:PRO:HA	1.97	0.46
1:A:236:ASP:O	1:A:239:GLU:HB3	2.15	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: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:B:344:THR:HA	1:B:362:ALA:HB1	1.97	0.46
1:A:16:ASP:O	1:A:20:GLY:N	2.49	0.46
1:A:371:MET:HB2	1:A:376:MET:HE3	1.96	0.46
1:A:94:ILE:HD12	1:B:205:ARG:NH1	2.31	0.46
1:A:431:LYS:HB2	1:A:432:GLU:OE1	2.15	0.46
1:A:289:ALA:O	1:B:111:ASN:HA	2.14	0.46
1:A:6:ARG:NH2	1:A:64:THR:HG23	2.31	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:400:ILE:HD13	1:B:435:ARG:NH2	2.31	0.45
1:B:50:SER:HB3	1:B:69: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:25:LEU:HD12	1:A:84:ALA:HB2	1.98	0.45
1:B:276:ARG:HB2	1:B:284:LEU:CD1	2.46	0.45
1:A:75:ASP:OD1	1:A:78:ARG:NH1	2.49	0.45
1:A:295:THR:HG23	1:A:305:ALA:CA	2.46	0.45
1:B:174:LYS:CB	1:B:175:PRO:CD	2.94	0.45
1:B:169:LEU:HD11	1:B:196:GLN:HA	1.97	0.45
1:A:455:LEU:HD12	1:A:455:LEU:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:OE1	1:A:121:ALA:O	2.35	0.45
1:B:448:TYR:O	1:B:451:TRP:HB3	2.16	0.45
1:B:7:TYR:O	1:B:70:LEU:HA	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:444:ALA:O	1:B:445:ASP:C	2.55	0.45
1:B:276:ARG:HB2	1:B:284:LEU:HD12	1.99	0.45
1:B:162:GLY:CA	1:B:189:PHE:O	2.61	0.44
1:A:291:HIS:HD2	1:A:291:HIS:H	1.47	0.44
1:A:431:LYS:HG3	1:A:431:LYS:H	1.39	0.44
1:A:295:THR:CG2	1:A:305:ALA:HB2	2.46	0.44
1:A:437:PHE:HB3	1:A:451:TRP:CZ3	2.52	0.44
1:A:337:ARG:NE	1:A:341:TYR:HE1	2.15	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:367:ILE:HG22	1:A:390:LEU:HD12	1.98	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:HA	1:A:101:ILE:HD12	1.97	0.44
1:B:101:ILE:HD11	1:B:311:MET:HG2	1.98	0.44
1:A:104:PHE:CE2	1:A:109:MET:HE2	2.52	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: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:128:VAL:HA	1:A:129:PRO:HD3	1.71	0.43
1:B:376:MET:CB	1:B:377:PRO:CD	2.89	0.43
1:B:322:THR:HG21	1:B:365:PRO:HB3	2.01	0.43
1:A:76:GLU:H	1:A:76:GLU:HG2	1.59	0.43
1:B:273:THR:O	1:B:273:THR:HG22	2.18	0.43
1:B:444:ALA:O	1:B:448:TYR:N	2.50	0.43
1:B:165:ILE:HD13	1:B:165:ILE:HA	1.94	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:336:ASP:HA	1:B:339:ILE:CB	2.47	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:A:191:LYS:HD2	1:A:285:HIS:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:HG3	1:A:135:LEU:O	2.19	0.43
1:B:436:ALA:O	1:B:439:SER:N	2.51	0.43
1:A:65:ARG:CG	1:A:65:ARG:O	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:B:159:LEU:HD12	1:B:160:VAL:N	2.34	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:A:168:LYS:HB2	1:A:193:ASP:OD1	2.19	0.42
1:A:337:ARG:HG2	1:A:337:ARG:O	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: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:150:LEU:CG	1:A:227:LEU:HD11	2.48	0.42
1:A:123:MET:CE	1:A:307:VAL:HG11	2.50	0.42
1:A:8:VAL:HG21	1:A:39:VAL:CG1	2.50	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:402:GLY:O	1:A:406:GLY:N	2.52	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:B:372:ASN:OD1	1:B:375:ARG:NH1	2.52	0.42
1:A:152:ARG:HB3	1:A:153:PRO:CD	2.48	0.42
1:B:372:ASN:O	1:B:376:MET:HE3	2.20	0.41
1:B:168:LYS:HG3	1:B:193:ASP:OD2	2.19	0.41
1:B:103:SER:O	1:B:107:LEU:HB2	2.20	0.41
1:B:424:LEU:HD23	1:B:454:ALA:CB	2.50	0.41
1:B:3:GLN:HE21	1:B:44:HIS:CG	2.38	0.41
1:A:399:HIS:HE1	1:A:435:ARG:HB3	1.85	0.41
1:B:334:SER:O	1:B:338:ALA:HB3	2.20	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:300:LYS:H	1:A:300:LYS:HG2	1.48	0.41
1:A:191:LYS:HD2	1:A:285:HIS:CE1	2.55	0.41
1:B:433:LEU:HA	1:B:433:LEU:HD12	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:B:336:ASP:HA	1:B:339:ILE:CG1	2.51	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:B:456:GLY:O	1:B:457:VAL:CB	2.63	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:A:25:LEU:HD22	1:A:127:TYR:HD1	1.86	0.41
1:A:261:LEU:HD11	1:A:287:HIS:HB2	2.02	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:B:244:GLY:HA3	1:B:279:PHE:CZ	2.56	0.41
1:B:159:LEU:HD12	1:B:160:VAL:H	1.86	0.40
1:B:45:PHE:CA	1:B:115:MET:HE3	2.43	0.40
1:B:184:TRP:HB3	1:B:226:LYS:HD3	2.03	0.40
1:A:139:PRO:HD3	1:A:313:ARG:O	2.21	0.40
1:B:41:THR:HG23	1:B:117:ASP:O	2.21	0.40
1:A:434:ALA:O	1:A:437:PHE:HB2	2.21	0.40
1:A:337:ARG:NE	1:A:341:TYR:CE1	2.88	0.40
1:A:336:ASP:HA	1:A:339:ILE:HD12	2.02	0.40
1:B:33:LYS:O	1:B:34:ALA:C	2.60	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:B:265:TYR:CZ	1:B:291:HIS:HA	2.56	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: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:B:366:ILE:HG21	1:B:366:ILE:HD13	1.85	0.40
1:A:278:ARG:CA	1:A:278:ARG:HE	2.09	0.40
1:B:172:ARG:HB3	1:B:172:ARG:HE	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%)	3 12
1	B	429/490 (88%)	365 (85%)	46 (11%)	18 (4%)	3 13
All	All	860/980 (88%)	739 (86%)	84 (10%)	37 (4%)	3 13

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

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 3
1	B	327/376 (87%)	276 (84%)	51 (16%)	3 10
All	All	657/752 (87%)	530 (81%)	127 (19%)	2 5

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

Some 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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	500	-	7,10,10	4.40	6 (85%)	7,14,14	2.97	6 (85%)
2	3PG	B	500	-	7,10,10	1.84	1 (14%)	7,14,14	1.35	0

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	A	500	-	-	0/6/10/10	0/0/0/0
2	3PG	B	500	-	-	0/6/10/10	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	3PG	P-O3P	2.38	1.63	1.54
2	A	500	3PG	P-O4P	2.78	1.64	1.54
2	B	500	3PG	P-O2P	3.07	1.61	1.51
2	A	500	3PG	P-O2P	3.46	1.62	1.51
2	A	500	3PG	O1P-C3	3.54	1.59	1.44
2	A	500	3PG	C3-C2	5.85	1.72	1.50
2	A	500	3PG	P-O1P	7.84	1.86	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	3PG	O3-C2-C1	-3.77	99.88	111.44
2	A	500	3PG	O4P-P-O2P	-2.79	101.61	110.58
2	A	500	3PG	O3P-P-O2P	-2.01	104.11	110.58
2	A	500	3PG	O4P-P-O1P	2.43	113.55	106.56
2	A	500	3PG	O3P-P-O1P	3.38	116.29	106.56
2	A	500	3PG	O1P-P-O2P	4.04	117.44	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.