Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 PM GMT

PDB ID	:	5RUB
Title	:	CRYSTALLOGRAPHIC REFINEMENT AND STRUCTURE OF RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE FROM RHODOSPIRILLUM RUBRUM AT 1.7 ANGSTROMS RESOLUTION
Authors	:	Schneider, G.; Lindqvist, Y.; Lundqvist, T.
Deposited on	:	1990-05-29
Resolution	:	1.70 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 ⓘ symbol.

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

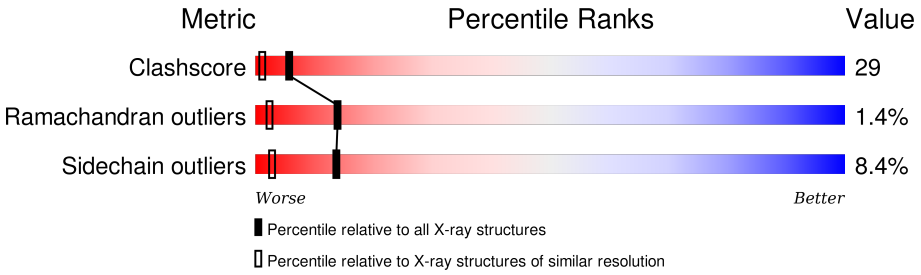
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.70 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	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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	50% 27% 11% • 11%
1	B	490	52% 27% 8% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7377 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	436	Total	C	N	O	S	18	0	0
			3330	2110	588	617	15			
1	B	433	Total	C	N	O	S	9	0	0
			3311	2100	585	611	15			

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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	342	Total	O	0	0
			342	342		
2	B	394	Total	O	0	0
			394	394		

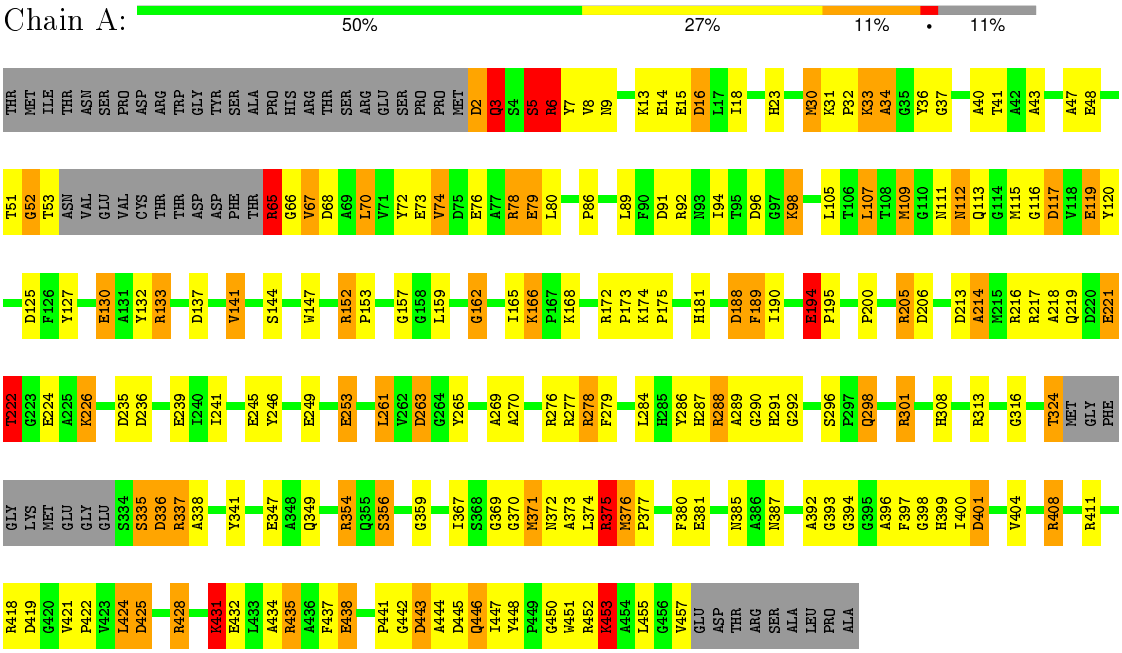
3 Residue-property plots (i)

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.

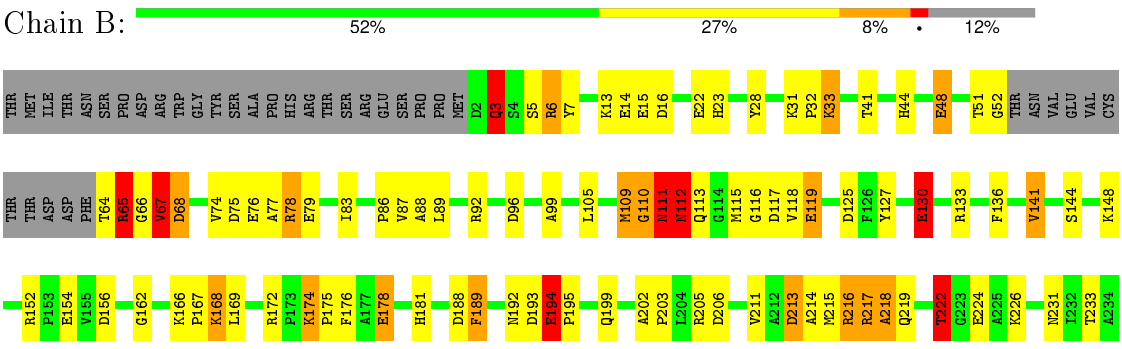
• Molecule 1: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)

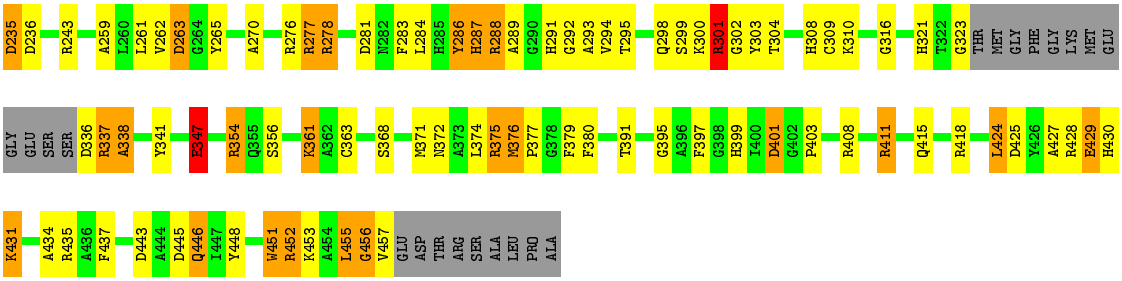
Chain A:



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

Chain B:




D235 D236 R243 A259 L260 L261 V262 D263 G264 Y265 A270 R276 R277 R278 D281 W282 F283 L284 H285 Y286 H287 R288 A289 G290 H291 G292 A293 V294 T295 Q298 S299 K300 R301 G302 Y303 T304 H308 C309 K310 G316 H321 T322 G323 THR MET GLY PHE GLY LYS MET GLU
GLY GLU SER SER D336 R337 A338 Y341 E347 R354 Q355 S356 K361 A362 C363 S368 M371 N372 A373 L374 R375 M376 P377 G378 F379 F380 T391 G395 A396 F397 G398 H399 I400 D401 G402 P403 R408 R411 Q415 R418 L424 D425 Y426 A427 R428 E429 H430
K431 A434 R435 A436 F437 D443 A444 D445 Q446 I447 Y448 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)	5.50 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (5.50-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.03	1/3410 (0.0%)	2.17	117/4620 (2.5%)
1	B	1.06	0/3391	2.10	114/4594 (2.5%)
All	All	1.04	1/6801 (0.0%)	2.14	231/9214 (2.5%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	GLU	CD-OE1	-6.28	1.18	1.25

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	236	ASP	CB-CG-OD1	20.44	136.70	118.30
1	A	288	ARG	NE-CZ-NH2	18.32	129.46	120.30
1	A	133	ARG	CD-NE-CZ	17.43	147.99	123.60
1	A	152	ARG	NE-CZ-NH2	-17.18	111.71	120.30
1	B	172	ARG	NE-CZ-NH1	17.03	128.81	120.30
1	A	133	ARG	NE-CZ-NH2	-16.61	112.00	120.30
1	B	301	ARG	NE-CZ-NH2	16.52	128.56	120.30
1	A	278	ARG	NE-CZ-NH1	16.48	128.54	120.30
1	B	96	ASP	CB-CG-OD1	15.54	132.29	118.30
1	B	276	ARG	NE-CZ-NH1	15.54	128.07	120.30
1	A	216	ARG	NE-CZ-NH2	-15.31	112.64	120.30
1	A	133	ARG	NE-CZ-NH1	14.87	127.74	120.30
1	A	428	ARG	NE-CZ-NH1	14.71	127.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ARG	NE-CZ-NH2	14.46	127.53	120.30
1	A	408	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	B	172	ARG	CD-NE-CZ	13.23	142.13	123.60
1	B	188	ASP	CB-CG-OD2	-12.91	106.68	118.30
1	A	194	GLU	OE1-CD-OE2	-12.83	107.91	123.30
1	B	276	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	A	205	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	A	16	ASP	CB-CG-OD2	-12.22	107.30	118.30
1	A	172	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	A	428	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	A	152	ARG	NH1-CZ-NH2	11.84	132.42	119.40
1	B	243	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	B	418	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	B	172	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	A	277	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	A	313	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	B	152	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	A	2	ASP	CB-CG-OD1	10.51	127.76	118.30
1	B	425	ASP	CB-CG-OD1	10.33	127.60	118.30
1	A	431	LYS	CA-CB-CG	10.30	136.05	113.40
1	A	313	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	B	217	ARG	NE-CZ-NH1	9.89	125.24	120.30
1	B	119	GLU	OE1-CD-OE2	9.81	135.08	123.30
1	B	188	ASP	CB-CG-OD1	9.67	127.01	118.30
1	B	347	GLU	OE1-CD-OE2	9.66	134.89	123.30
1	A	152	ARG	NE-CZ-NH1	-9.53	115.54	120.30
1	A	92	ARG	NE-CZ-NH1	-9.49	115.56	120.30
1	B	401	ASP	CB-CG-OD1	9.49	126.84	118.30
1	A	276	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	B	452	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	B	337	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	A	435	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	B	14	GLU	CG-CD-OE1	9.12	136.55	118.30
1	A	213	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	B	278	ARG	NE-CZ-NH2	9.07	124.84	120.30
1	B	236	ASP	OD1-CG-OD2	-9.07	106.07	123.30
1	B	156	ASP	CB-CG-OD1	9.06	126.45	118.30
1	B	452	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	B	263	ASP	CB-CG-OD1	8.84	126.25	118.30
1	B	206	ASP	CB-CG-OD1	8.79	126.21	118.30
1	B	263	ASP	CB-CG-OD2	-8.69	110.48	118.30
1	B	194	GLU	CG-CD-OE1	8.67	135.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	235	ASP	CB-CG-OD1	8.67	126.10	118.30
1	B	429	GLU	CA-CB-CG	8.66	132.44	113.40
1	A	213	ASP	CB-CG-OD1	8.61	126.05	118.30
1	A	453	LYS	CA-CB-CG	8.59	132.29	113.40
1	B	144	SER	CB-CA-C	8.27	125.82	110.10
1	A	194	GLU	CG-CD-OE1	8.25	134.80	118.30
1	A	288	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	A	425	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	A	6	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	A	16	ASP	CB-CG-OD1	8.06	125.56	118.30
1	A	206	ASP	CB-CG-OD1	8.04	125.53	118.30
1	B	316	GLY	CA-C-O	-7.93	106.33	120.60
1	B	337	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	347	GLU	OE1-CD-OE2	7.90	132.78	123.30
1	A	419	ASP	CB-CG-OD2	7.89	125.41	118.30
1	A	408	ARG	NH1-CZ-NH2	7.87	128.06	119.40
1	A	14	GLU	CG-CD-OE1	7.87	134.04	118.30
1	A	411	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	B	68	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	411	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	236	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	205	ARG	CD-NE-CZ	-7.67	112.86	123.60
1	A	127	TYR	CB-CG-CD1	7.67	125.60	121.00
1	B	14	GLU	OE1-CD-OE2	-7.64	114.14	123.30
1	B	218	ALA	N-CA-CB	7.60	120.74	110.10
1	A	278	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	130	GLU	OE1-CD-OE2	-7.55	114.24	123.30
1	B	401	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	B	66	GLY	N-CA-C	-7.48	94.41	113.10
1	B	235	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	A	194	GLU	CA-CB-CG	7.39	129.66	113.40
1	A	127	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	A	125	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	381	GLU	CG-CD-OE2	-7.30	103.69	118.30
1	A	216	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	281	ASP	CB-CG-OD1	7.23	124.80	118.30
1	B	96	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	451	TRP	CA-CB-CG	7.18	127.35	113.70
1	A	354	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	B	130	GLU	OE1-CD-OE2	-7.11	114.76	123.30
1	B	119	GLU	CG-CD-OE2	-7.05	104.21	118.30
1	B	67	VAL	CB-CA-C	7.01	124.73	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	213	ASP	CB-CG-OD2	6.95	124.56	118.30
1	B	278	ARG	NH1-CZ-NH2	-6.93	111.78	119.40
1	B	92	ARG	CB-CA-C	6.87	124.14	110.40
1	B	119	GLU	CA-CB-CG	-6.84	98.36	113.40
1	A	205	ARG	NH1-CZ-NH2	6.78	126.86	119.40
1	B	222	THR	N-CA-CB	-6.74	97.49	110.30
1	B	411	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	A	141	VAL	N-CA-CB	-6.65	96.87	111.50
1	A	288	ARG	CD-NE-CZ	-6.63	114.31	123.60
1	A	65	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	B	65	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	B	395	GLY	N-CA-C	-6.58	96.64	113.10
1	B	16	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	408	ARG	CD-NE-CZ	-6.51	114.48	123.60
1	A	34	ALA	N-CA-CB	-6.49	101.01	110.10
1	B	194	GLU	CG-CD-OE2	-6.49	105.33	118.30
1	A	14	GLU	CG-CD-OE2	-6.46	105.37	118.30
1	B	109	MET	N-CA-CB	-6.40	99.08	110.60
1	B	99	ALA	O-C-N	-6.39	112.47	122.70
1	B	193	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	72	TYR	CB-CG-CD2	6.36	124.82	121.00
1	B	347	GLU	CG-CD-OE2	-6.35	105.61	118.30
1	A	298	GLN	N-CA-CB	6.34	122.02	110.60
1	B	411	ARG	CG-CD-NE	6.31	125.04	111.80
1	A	288	ARG	N-CA-CB	-6.27	99.31	110.60
1	B	141	VAL	N-CA-CB	-6.26	97.72	111.50
1	B	408	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	B	216	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	189	PHE	N-CA-CB	-6.21	99.43	110.60
1	B	199	GLN	CA-CB-CG	6.20	127.03	113.40
1	B	127	TYR	CB-CG-CD2	6.19	124.71	121.00
1	A	381	GLU	CG-CD-OE1	6.18	130.66	118.30
1	A	239	GLU	N-CA-CB	6.18	121.72	110.60
1	B	278	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	72	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	A	2	ASP	CA-CB-CG	6.14	126.90	113.40
1	B	288	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	B	338	ALA	N-CA-CB	6.08	118.61	110.10
1	A	8	VAL	CA-CB-CG2	6.07	120.01	110.90
1	A	435	ARG	NH1-CZ-NH2	-6.05	112.75	119.40
1	B	92	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	117	ASP	CB-CG-OD2	6.03	123.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	356	SER	N-CA-CB	6.03	119.54	110.50
1	B	375	ARG	CD-NE-CZ	6.02	132.03	123.60
1	B	259	ALA	N-CA-CB	6.01	118.51	110.10
1	B	152	ARG	NH1-CZ-NH2	5.96	125.95	119.40
1	B	127	TYR	CB-CG-CD1	-5.95	117.43	121.00
1	A	74	VAL	CA-CB-CG1	5.92	119.78	110.90
1	B	130	GLU	CG-CD-OE1	5.91	130.12	118.30
1	B	6	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	91	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	125	ASP	OD1-CG-OD2	-5.88	112.14	123.30
1	A	98	LYS	CA-CB-CG	-5.87	100.49	113.40
1	A	347	GLU	N-CA-CB	-5.86	100.06	110.60
1	A	298	GLN	CB-CG-CD	5.84	126.79	111.60
1	A	70	LEU	CB-CG-CD2	-5.82	101.10	111.00
1	B	65	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	B	287	HIS	CA-CB-CG	-5.75	103.83	113.60
1	A	30	MET	CA-CB-CG	5.72	123.03	113.30
1	A	96	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	445	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	96	ASP	CA-C-N	5.71	127.63	116.20
1	A	194	GLU	CB-CG-CD	5.71	129.60	114.20
1	A	65	ARG	O-C-N	5.70	132.90	123.20
1	B	288	ARG	CG-CD-NE	5.70	123.77	111.80
1	A	401	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	78	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	304	THR	CA-CB-OG1	-5.68	97.07	109.00
1	B	361	LYS	CB-CA-C	5.68	121.77	110.40
1	B	277	ARG	CD-NE-CZ	-5.67	115.66	123.60
1	B	77	ALA	CB-CA-C	5.67	118.61	110.10
1	A	432	GLU	CG-CD-OE1	5.67	129.64	118.30
1	A	67	VAL	CB-CA-C	5.67	122.16	111.40
1	B	288	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	A	425	ASP	CA-CB-CG	-5.63	101.01	113.40
1	A	269	ALA	CB-CA-C	5.63	118.55	110.10
1	A	188	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	337	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	3	GLN	CA-C-O	5.57	131.79	120.10
1	B	174	LYS	CD-CE-NZ	-5.55	98.94	111.70
1	B	435	ARG	CD-NE-CZ	-5.54	115.85	123.60
1	B	78	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	286	TYR	CB-CG-CD1	5.49	124.29	121.00
1	A	65	ARG	C-N-CA	5.48	133.81	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	GLU	CG-CD-OE1	5.47	129.24	118.30
1	A	119	GLU	N-CA-CB	5.42	120.35	110.60
1	A	190	ILE	O-C-N	5.41	131.36	122.70
1	A	277	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	B	68	ASP	O-C-N	5.37	131.30	122.70
1	A	226	LYS	O-C-N	5.34	131.25	122.70
1	B	262	VAL	CA-CB-CG2	5.32	118.88	110.90
1	A	263	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	152	ARG	CD-NE-CZ	-5.29	116.20	123.60
1	A	261	LEU	O-C-N	5.28	131.15	122.70
1	A	418	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	337	ARG	N-CA-CB	5.26	120.07	110.60
1	A	144	SER	CB-CA-C	5.26	120.09	110.10
1	B	361	LYS	CD-CE-NZ	-5.25	99.61	111.70
1	B	391	THR	N-CA-C	-5.25	96.83	111.00
1	B	301	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	174	LYS	CB-CA-C	5.24	120.87	110.40
1	A	438	GLU	CA-CB-CG	5.23	124.91	113.40
1	B	277	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	B	110	GLY	CA-C-O	5.19	129.94	120.60
1	B	301	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	A	375	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	B	276	ARG	O-C-N	-5.18	114.42	122.70
1	A	189	PHE	N-CA-CB	-5.17	101.30	110.60
1	A	125	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	435	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	354	ARG	CD-NE-CZ	-5.12	116.43	123.60
1	A	222	THR	N-CA-CB	-5.12	100.58	110.30
1	A	336	ASP	N-CA-CB	5.12	119.81	110.60
1	A	316	GLY	CA-C-O	-5.11	111.41	120.60
1	A	288	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	A	162	GLY	CA-C-O	5.10	129.78	120.60
1	A	239	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	B	430	HIS	CA-CB-CG	-5.08	104.97	113.60
1	A	428	ARG	CG-CD-NE	5.07	122.46	111.80
1	B	222	THR	OG1-CB-CG2	5.07	121.67	110.00
1	A	214	ALA	N-CA-CB	5.07	117.20	110.10
1	A	137	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	79	GLU	CG-CD-OE1	5.05	128.39	118.30
1	B	178	GLU	CG-CD-OE1	5.05	128.39	118.30
1	A	79	GLU	CA-CB-CG	5.04	124.50	113.40
1	A	132	TYR	CB-CG-CD2	-5.04	117.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	283	PHE	CB-CG-CD2	5.04	124.33	120.80
1	B	363	CYS	N-CA-C	-5.04	97.39	111.00
1	A	279	PHE	CZ-CE2-CD2	-5.04	114.06	120.10
1	B	288	ARG	N-CA-CB	-5.03	101.54	110.60
1	A	253	GLU	CA-CB-CG	5.03	124.47	113.40
1	B	125	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	111	ASN	OD1-CG-ND2	5.03	133.46	121.90
1	B	408	ARG	NH1-CZ-NH2	5.03	124.93	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	277	ARG	Sidechain

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	3330	0	3233	192	1
1	B	3311	0	3216	206	0
2	A	342	0	0	31	0
2	B	394	0	0	29	0
All	All	7377	0	6449	379	1

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 29.

All (379) 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:2:ASP:O	1:A:3:GLN:HG3	1.36	1.24
1:B:337:ARG:HD2	1:B:341:TYR:CZ	1.79	1.18
1:A:194:GLU:HG3	1:A:195:PRO:HD3	1.31	1.11
1:B:456:GLY:O	1:B:457:VAL:HG23	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:HB3	1:A:6:ARG:HB3	1.35	1.07
1:B:194:GLU:OE1	1:B:195:PRO:HG3	1.59	1.01
1:B:263:ASP:OD2	1:B:289:ALA:HB3	1.60	0.99
1:B:299:SER:HA	1:B:301:ARG:NH1	1.76	0.99
1:B:112:ASN:ND2	1:B:112:ASN:H	1.56	0.98
1:B:64:THR:HG22	1:B:65:ARG:H	1.29	0.98
1:A:2:ASP:O	1:A:3:GLN:CG	2.11	0.98
1:B:299:SER:HA	1:B:301:ARG:HH12	1.26	0.97
1:B:65:ARG:HD2	1:B:86:PRO:HB3	1.45	0.97
1:A:194:GLU:CG	1:A:195:PRO:HD3	1.94	0.96
1:A:263:ASP:OD1	1:A:289:ALA:HB3	1.64	0.96
1:B:337:ARG:HG2	1:B:337:ARG:O	1.68	0.93
1:B:111:ASN:O	1:B:113:GLN:N	2.00	0.93
1:A:385:ASN:HD22	1:A:387:ASN:H	1.17	0.92
1:B:112:ASN:H	1:B:112:ASN:HD22	1.19	0.91
1:B:411:ARG:NH1	2:B:815:HOH:O	2.05	0.89
1:B:65:ARG:CD	1:B:86:PRO:HB3	2.01	0.89
1:B:41:THR:CG2	1:B:118:VAL:HG22	2.03	0.88
1:B:15:GLU:HG2	2:B:809:HOH:O	1.74	0.87
1:B:213:ASP:HB3	2:B:777:HOH:O	1.75	0.87
1:A:52:GLY:H	1:B:168:LYS:H	1.19	0.86
1:A:105:LEU:HD23	1:A:109:MET:HE2	1.56	0.86
1:B:64:THR:HG22	1:B:65:ARG:N	1.89	0.86
1:A:371:MET:SD	1:A:375:ARG:HB3	2.16	0.85
1:B:65:ARG:HD3	1:B:86:PRO:HA	1.56	0.85
1:A:253:GLU:HG2	2:A:687:HOH:O	1.74	0.84
1:A:65:ARG:N	2:A:506:HOH:O	2.11	0.83
1:A:222:THR:HG23	1:A:224:GLU:HB2	1.61	0.83
1:A:105:LEU:HD23	1:A:109:MET:CE	2.08	0.83
1:A:424:LEU:HD21	1:A:448:TYR:HB3	1.62	0.82
1:A:424:LEU:HD22	1:A:448:TYR:CD1	2.13	0.82
1:B:376:MET:HB3	1:B:377:PRO:HD3	1.59	0.82
1:B:111:ASN:C	1:B:113:GLN:H	1.81	0.82
1:B:222:THR:HG22	1:B:224:GLU:H	1.42	0.81
1:B:52:GLY:HA3	2:B:845:HOH:O	1.80	0.81
1:A:370:GLY:HA3	1:A:396:ALA:HB2	1.63	0.81
1:B:41:THR:HG22	1:B:118:VAL:HG22	1.63	0.80
1:A:450:GLY:O	1:A:453:LYS:HB3	1.81	0.80
1:A:222:THR:CG2	1:A:224:GLU:HB2	2.11	0.80
1:B:456:GLY:O	1:B:457:VAL:CG2	2.30	0.80
1:A:52:GLY:N	1:B:168:LYS:H	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HG22	1:A:224:GLU:H	1.47	0.79
1:A:65:ARG:HA	1:A:70:LEU:HD11	1.65	0.79
1:A:33:LYS:HG3	1:A:117:ASP:HA	1.63	0.79
1:B:194:GLU:OE1	1:B:195:PRO:CG	2.31	0.79
1:B:222:THR:CG2	1:B:224:GLU:H	1.96	0.79
1:B:65:ARG:NH1	1:B:88:ALA:H	1.81	0.78
1:B:52:GLY:CA	2:B:845:HOH:O	2.32	0.78
1:B:222:THR:HG23	1:B:224:GLU:HB2	1.66	0.77
1:A:194:GLU:HG3	1:A:195:PRO:CD	2.13	0.77
1:A:438:GLU:O	1:A:441:PRO:HD3	1.83	0.77
1:B:76:GLU:O	2:B:591:HOH:O	2.02	0.77
1:B:105:LEU:O	1:B:109:MET:HB3	1.84	0.77
1:B:337:ARG:HD2	1:B:341:TYR:OH	1.84	0.77
1:B:65:ARG:HH11	1:B:86:PRO:CB	1.98	0.76
1:B:23:HIS:NE2	1:B:65:ARG:HG2	2.00	0.76
1:B:431:LYS:HB2	1:B:431:LYS:NZ	1.99	0.76
1:B:194:GLU:CD	1:B:195:PRO:HD3	2.05	0.76
1:A:107:LEU:CD1	1:B:195:PRO:HB3	2.16	0.76
1:A:52:GLY:H	1:B:168:LYS:N	1.83	0.75
1:B:424:LEU:O	1:B:428:ARG:HG3	1.86	0.75
1:A:119:GLU:O	1:A:301:ARG:NH2	2.20	0.75
1:B:337:ARG:CD	1:B:341:TYR:CZ	2.68	0.75
1:A:452:ARG:HG2	1:A:457:VAL:HG23	1.68	0.74
1:A:324:THR:HG23	1:A:367:ILE:HG21	1.69	0.74
1:B:205:ARG:HD2	2:B:829:HOH:O	1.87	0.74
1:B:399:HIS:CE1	1:B:401:ASP:HB2	2.22	0.74
1:B:376:MET:HE2	1:B:376:MET:HA	1.68	0.73
1:A:425:ASP:HA	1:A:428:ARG:HD3	1.70	0.73
1:A:371:MET:CE	1:A:375:ARG:HD3	2.18	0.73
1:A:33:LYS:HE3	1:A:116:GLY:O	1.88	0.73
1:A:2:ASP:C	1:A:3:GLN:HG3	2.09	0.73
1:A:376:MET:HB3	1:A:377:PRO:HD3	1.71	0.73
1:B:48:GLU:HB2	1:B:115:MET:HE1	1.70	0.72
1:A:218:ALA:O	1:A:222:THR:HB	1.90	0.72
1:B:231:ASN:ND2	2:B:537:HOH:O	2.23	0.71
1:B:375:ARG:NH1	1:B:443:ASP:OD1	2.23	0.71
1:A:194:GLU:OE1	1:B:111:ASN:HB2	1.90	0.71
1:B:337:ARG:CG	1:B:337:ARG:O	2.38	0.70
1:A:222:THR:CG2	1:A:224:GLU:H	2.04	0.70
1:A:15:GLU:HG3	2:A:565:HOH:O	1.90	0.70
1:B:23:HIS:CE1	1:B:65:ARG:HG2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ASN:HD21	1:B:375:ARG:HH11	1.40	0.70
1:B:452:ARG:NH1	2:B:860:HOH:O	2.15	0.70
1:A:13:LYS:O	1:A:16:ASP:HB2	1.92	0.69
1:A:2:ASP:O	1:A:3:GLN:CB	2.40	0.69
1:B:428:ARG:HH11	1:B:428:ARG:CB	2.04	0.69
1:B:44:HIS:CG	1:B:115:MET:HE2	2.27	0.69
1:B:112:ASN:ND2	1:B:112:ASN:N	2.35	0.69
1:B:65:ARG:HH12	1:B:88:ALA:CB	2.07	0.68
1:B:130:GLU:H	1:B:130:GLU:CD	1.95	0.68
1:B:372:ASN:ND2	1:B:375:ARG:HH11	1.91	0.68
1:B:65:ARG:HH12	1:B:88:ALA:H	1.40	0.68
1:B:218:ALA:O	1:B:222:THR:HB	1.94	0.68
1:A:290:GLY:C	1:A:292:GLY:H	1.96	0.67
1:B:222:THR:CG2	1:B:224:GLU:HB2	2.24	0.67
1:B:52:GLY:C	2:B:845:HOH:O	2.33	0.67
1:B:424:LEU:HD12	1:B:455:LEU:CD1	2.25	0.67
1:A:52:GLY:CA	1:B:168:LYS:H	2.08	0.66
1:A:349:GLN:OE1	1:A:354:ARG:NE	2.23	0.66
1:A:371:MET:HE2	1:A:375:ARG:HD3	1.77	0.66
1:B:376:MET:CA	1:B:376:MET:HE2	2.24	0.66
1:B:112:ASN:HB2	2:B:858:HOH:O	1.95	0.65
1:B:64:THR:CG2	1:B:65:ARG:N	2.56	0.65
1:A:376:MET:HE2	1:A:376:MET:HA	1.78	0.65
1:A:265:TYR:CZ	1:A:291:HIS:HA	2.31	0.65
1:A:452:ARG:HA	1:A:457:VAL:CG2	2.27	0.65
1:B:424:LEU:HD12	1:B:455:LEU:HD11	1.79	0.65
1:B:75:ASP:OD1	1:B:78:ARG:HG3	1.96	0.65
1:B:65:ARG:HD3	1:B:86:PRO:CA	2.27	0.64
1:A:288:ARG:O	1:A:291:HIS:HD2	1.80	0.64
1:A:288:ARG:O	1:A:291:HIS:CD2	2.50	0.64
1:A:112:ASN:HD22	1:A:112:ASN:C	1.99	0.64
1:B:148:LYS:HD2	1:B:154:GLU:OE1	1.97	0.64
1:B:65:ARG:HH11	1:B:86:PRO:HB3	1.60	0.64
1:B:217:ARG:NH2	2:B:714:HOH:O	2.30	0.64
1:A:73:GLU:OE2	2:A:472:HOH:O	2.15	0.64
1:A:3:GLN:HB3	1:A:6:ARG:CB	2.21	0.63
1:A:194:GLU:CB	1:A:195:PRO:HD3	2.28	0.63
1:A:337:ARG:O	1:A:341:TYR:CD1	2.52	0.63
1:A:356:SER:HB3	2:A:494:HOH:O	1.98	0.63
1:A:107:LEU:HD11	1:B:195:PRO:CB	2.28	0.63
1:A:349:GLN:OE1	1:A:354:ARG:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:HB2	1:A:115:MET:HE3	1.81	0.62
1:B:65:ARG:HH12	1:B:88:ALA:HB3	1.65	0.62
1:A:451:TRP:O	1:A:455:LEU:HD13	2.00	0.62
1:A:74:VAL:HA	1:A:80:LEU:O	1.99	0.62
1:A:78:ARG:HE	1:A:80:LEU:HD22	1.64	0.62
1:A:107:LEU:HD11	1:B:195:PRO:HB3	1.80	0.61
1:A:111:ASN:ND2	1:B:194:GLU:HG2	2.15	0.61
1:B:287:HIS:CD2	2:B:750:HOH:O	2.52	0.61
1:B:288:ARG:NH2	1:B:291:HIS:NE2	2.48	0.61
1:B:130:GLU:OE1	2:B:532:HOH:O	2.16	0.61
1:B:194:GLU:OE1	1:B:195:PRO:HD3	2.00	0.61
1:A:105:LEU:CD2	1:A:109:MET:HE2	2.30	0.61
1:B:337:ARG:HG3	1:B:341:TYR:CE2	2.36	0.61
1:A:369:GLY:O	1:A:392:ALA:HA	2.01	0.60
1:A:424:LEU:HD22	1:A:448:TYR:HD1	1.63	0.60
1:A:133:ARG:NH2	2:A:510:HOH:O	2.06	0.59
1:A:443:ASP:O	1:A:447:ILE:HG12	2.02	0.59
1:A:424:LEU:CD2	1:A:448:TYR:HB3	2.31	0.59
1:A:18:ILE:HG22	2:A:598:HOH:O	2.01	0.59
1:B:194:GLU:OE1	1:B:195:PRO:CD	2.51	0.59
1:A:424:LEU:CD2	1:A:448:TYR:CD1	2.85	0.59
1:B:376:MET:HG3	1:B:380:PHE:CE2	2.37	0.59
1:A:105:LEU:CD2	1:A:109:MET:CE	2.79	0.59
1:A:422:PRO:HD2	2:A:586:HOH:O	2.02	0.59
1:A:424:LEU:CD2	1:A:448:TYR:HD1	2.16	0.59
1:A:65:ARG:N	1:A:68:ASP:HB2	2.16	0.59
1:A:288:ARG:NH2	1:A:291:HIS:CE1	2.71	0.59
1:A:235:ASP:O	1:B:270:ALA:HA	2.03	0.59
1:B:321:HIS:CE1	1:B:323:GLY:HA2	2.38	0.58
1:A:67:VAL:O	1:A:89:LEU:HD11	2.04	0.58
1:A:288:ARG:HE	1:A:308:HIS:CD2	2.21	0.58
1:B:427:ALA:O	1:B:434:ALA:HB2	2.04	0.58
1:B:119:GLU:O	1:B:119:GLU:HG2	2.03	0.58
1:A:445:ASP:OD2	1:A:452:ARG:NH2	2.37	0.58
1:B:65:ARG:HD3	1:B:86:PRO:HB3	1.81	0.58
1:A:263:ASP:OD1	1:A:289:ALA:CB	2.46	0.58
1:A:324:THR:HG23	1:A:367:ILE:CG2	2.34	0.58
1:B:295:THR:HA	1:B:303:TYR:O	2.03	0.57
1:B:424:LEU:HD13	1:B:437:PHE:CZ	2.39	0.57
1:B:337:ARG:HD2	1:B:341:TYR:CE1	2.34	0.57
1:B:194:GLU:HB3	2:B:750:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ARG:NH2	1:B:291:HIS:CD2	2.72	0.57
1:A:52:GLY:HA3	1:B:168:LYS:H	1.68	0.57
1:A:48:GLU:HG3	1:A:115:MET:HE2	1.86	0.57
1:A:152:ARG:HB3	1:A:153:PRO:HD2	1.85	0.57
1:A:205:ARG:HD2	2:A:719:HOH:O	2.05	0.56
1:B:299:SER:CA	1:B:301:ARG:NH1	2.62	0.56
1:A:265:TYR:CE2	1:A:291:HIS:HA	2.40	0.56
1:A:422:PRO:CD	2:A:586:HOH:O	2.54	0.56
1:B:23:HIS:HD2	2:B:604:HOH:O	1.88	0.56
1:B:288:ARG:O	1:B:289:ALA:C	2.45	0.56
1:B:321:HIS:CE1	1:B:368:SER:OG	2.59	0.55
1:A:278:ARG:CD	2:A:760:HOH:O	2.53	0.55
1:B:41:THR:CG2	1:B:118:VAL:CG2	2.79	0.55
1:B:65:ARG:NH2	2:B:647:HOH:O	1.72	0.55
1:B:111:ASN:HB3	1:B:112:ASN:HD22	1.71	0.55
1:A:173:PRO:HG2	2:A:606:HOH:O	2.06	0.55
1:A:66:GLY:HA3	2:A:605:HOH:O	2.06	0.54
1:A:222:THR:HG21	1:A:226:LYS:CE	2.37	0.54
1:A:370:GLY:CA	1:A:396:ALA:HB2	2.36	0.54
1:A:394:GLY:HA2	1:A:397:PHE:HD1	1.71	0.54
1:B:347:GLU:OE2	1:B:354:ARG:NH1	2.40	0.54
1:B:65:ARG:HD3	1:B:86:PRO:CB	2.38	0.54
1:A:421:VAL:HG13	1:A:422:PRO:HD2	1.89	0.54
1:B:222:THR:HG23	1:B:224:GLU:CB	2.35	0.54
1:B:321:HIS:HE1	1:B:368:SER:OG	1.91	0.54
1:A:292:GLY:O	1:A:296:SER:HB2	2.08	0.54
1:A:404:VAL:O	1:A:408:ARG:HD2	2.08	0.54
1:B:67:VAL:O	1:B:89:LEU:HD21	2.08	0.53
1:B:178:GLU:OE1	1:B:217:ARG:NH2	2.40	0.53
1:A:335:SER:O	1:A:338:ALA:HB3	2.08	0.53
1:A:33:LYS:HB2	1:A:36:TYR:CD2	2.42	0.53
1:B:265:TYR:CZ	1:B:291:HIS:HA	2.43	0.53
1:A:431:LYS:HB2	2:A:662:HOH:O	2.07	0.53
1:B:337:ARG:CG	1:B:341:TYR:CE2	2.92	0.53
1:B:111:ASN:C	1:B:113:GLN:N	2.49	0.53
1:B:28:TYR:CE2	1:B:83:ILE:HD12	2.43	0.53
1:A:452:ARG:HA	1:A:457:VAL:HG23	1.89	0.52
1:B:23:HIS:HE1	1:B:64:THR:O	1.93	0.52
1:B:428:ARG:HB3	1:B:428:ARG:HH11	1.73	0.52
1:B:22:GLU:HB2	1:B:65:ARG:HE	1.73	0.52
1:A:444:ALA:O	1:A:448:TYR:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:MET:HB3	1:B:376:MET:HE1	1.90	0.52
1:A:222:THR:HG23	1:A:224:GLU:CB	2.38	0.52
1:B:51:THR:CG2	1:B:67:VAL:HG12	2.40	0.52
1:B:222:THR:CG2	1:B:224:GLU:N	2.70	0.52
1:B:446:GLN:C	1:B:446:GLN:HE21	2.13	0.52
1:B:65:ARG:CD	1:B:86:PRO:CB	2.83	0.52
1:A:174:LYS:HB3	1:A:175:PRO:HD3	1.92	0.52
1:B:6:ARG:HD3	1:B:7:TYR:CE2	2.45	0.52
1:B:194:GLU:CB	2:B:750:HOH:O	2.58	0.51
1:A:401:ASP:OD2	1:A:435:ARG:HG3	2.11	0.51
1:A:188:ASP:OD2	2:A:481:HOH:O	2.19	0.51
1:B:194:GLU:CG	1:B:195:PRO:HD3	2.41	0.51
1:A:287:HIS:HD2	1:A:288:ARG:N	2.09	0.51
1:A:408:ARG:NH2	2:A:536:HOH:O	2.44	0.51
1:A:98:LYS:NZ	2:A:774:HOH:O	2.44	0.51
1:B:166:LYS:HA	1:B:167:PRO:C	2.32	0.51
1:B:64:THR:CG2	1:B:65:ARG:H	2.01	0.51
1:A:37:GLY:O	1:A:41:THR:OG1	2.20	0.51
1:A:13:LYS:HB2	1:A:16:ASP:OD1	2.10	0.51
1:A:53:THR:H	1:B:167:PRO:HA	1.76	0.51
1:B:291:HIS:O	1:B:293:ALA:N	2.44	0.50
1:A:113:GLN:NE2	2:A:747:HOH:O	2.43	0.50
1:B:372:ASN:HD21	1:B:375:ARG:NH1	2.04	0.50
1:A:278:ARG:HD3	2:A:760:HOH:O	2.11	0.50
1:B:261:LEU:HD11	1:B:287:HIS:HB2	1.93	0.50
1:A:372:ASN:OD1	1:A:374:LEU:HB2	2.12	0.50
1:A:73:GLU:O	1:A:74:VAL:HG23	2.11	0.50
1:A:79:GLU:OE2	1:A:120:TYR:OH	2.21	0.50
1:A:278:ARG:HD2	2:A:760:HOH:O	2.10	0.50
1:B:133:ARG:NH1	2:B:717:HOH:O	2.17	0.49
1:B:168:LYS:HE2	1:B:194:GLU:OE2	2.12	0.49
1:A:200:PRO:HD2	1:B:88:ALA:O	2.12	0.49
1:A:33:LYS:HG3	1:A:117:ASP:CA	2.38	0.49
1:A:162:GLY:HA2	1:A:189:PHE:O	2.12	0.49
1:A:65:ARG:O	1:A:68:ASP:O	2.31	0.49
1:B:424:LEU:HD12	1:B:455:LEU:HD13	1.95	0.49
1:A:337:ARG:HG2	1:A:341:TYR:CZ	2.48	0.49
1:B:174:LYS:HB3	1:B:175:PRO:HD3	1.95	0.49
1:A:261:LEU:HD11	1:A:287:HIS:HB2	1.95	0.48
1:A:442:GLY:O	1:A:446:GLN:HG2	2.13	0.48
1:A:48:GLU:HG3	1:A:115:MET:CE	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HD12	1:B:205:ARG:NH1	2.28	0.48
1:B:215:MET:O	1:B:219:GLN:HG3	2.12	0.48
1:B:399:HIS:ND1	1:B:401:ASP:HB2	2.28	0.48
1:B:44:HIS:ND1	1:B:115:MET:HE2	2.28	0.48
1:A:376:MET:N	1:A:377:PRO:CD	2.77	0.48
1:A:222:THR:HG21	1:A:226:LYS:HE3	1.96	0.48
1:B:321:HIS:HB2	2:B:599:HOH:O	2.14	0.48
1:A:398:GLY:HA3	2:A:624:HOH:O	2.14	0.48
1:A:194:GLU:CB	1:A:195:PRO:CD	2.92	0.47
1:A:371:MET:CE	2:A:743:HOH:O	2.62	0.47
1:A:371:MET:SD	1:A:375:ARG:CB	2.96	0.47
1:A:165:ILE:O	1:A:166:LYS:HD3	2.14	0.47
1:B:448:TYR:O	1:B:451:TRP:HB3	2.14	0.47
1:B:428:ARG:NH1	1:B:428:ARG:CB	2.76	0.47
1:A:424:LEU:HD11	1:A:451:TRP:HA	1.96	0.47
1:B:65:ARG:NH2	1:B:87:VAL:HG23	2.29	0.47
1:B:336:ASP:C	1:B:338:ALA:N	2.67	0.47
1:A:270:ALA:HA	1:B:235:ASP:O	2.15	0.47
1:A:438:GLU:HG3	2:A:709:HOH:O	2.15	0.47
1:A:376:MET:HB2	1:A:376:MET:HE3	1.75	0.47
1:A:385:ASN:HD22	1:A:387:ASN:N	1.99	0.47
1:B:213:ASP:HB3	2:B:702:HOH:O	2.15	0.47
1:B:23:HIS:HE1	1:B:64:THR:C	2.19	0.46
1:A:48:GLU:CB	1:A:115:MET:HE3	2.46	0.46
1:A:435:ARG:NH1	1:A:438:GLU:OE1	2.48	0.46
1:B:148:LYS:HD2	1:B:154:GLU:CD	2.35	0.46
1:B:222:THR:HG21	1:B:226:LYS:CE	2.45	0.46
1:B:44:HIS:CE1	1:B:115:MET:CE	2.99	0.46
1:B:222:THR:HG23	1:B:224:GLU:N	2.31	0.46
1:B:194:GLU:CG	2:B:750:HOH:O	2.64	0.46
1:B:397:PHE:CD1	1:B:403:PRO:HG3	2.51	0.46
1:B:222:THR:HG21	1:B:226:LYS:HE3	1.97	0.46
1:B:288:ARG:NH1	1:B:308:HIS:CD2	2.84	0.46
1:A:51:THR:HG22	1:B:169:LEU:O	2.15	0.45
1:A:3:GLN:NE2	1:A:6:ARG:HH11	2.14	0.45
1:A:291:HIS:CD2	2:A:639:HOH:O	2.69	0.45
1:B:354:ARG:NH2	2:B:542:HOH:O	2.47	0.45
1:A:7:TYR:CE1	1:A:47:ALA:HA	2.51	0.45
1:A:241:ILE:O	1:A:245:GLU:HG3	2.16	0.45
1:A:107:LEU:CD1	1:B:195:PRO:CB	2.88	0.45
1:B:75:ASP:CG	1:B:78:ARG:HG3	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:HG21	1:B:67:VAL:HG12	1.99	0.45
1:A:2:ASP:O	1:A:3:GLN:HB2	2.17	0.45
1:B:265:TYR:CE1	1:B:291:HIS:HA	2.51	0.45
1:B:300:LYS:C	1:B:301:ARG:HG3	2.29	0.45
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.99	0.45
1:B:202:ALA:N	1:B:203:PRO:HD3	2.32	0.45
1:A:371:MET:HE1	2:A:743:HOH:O	2.17	0.45
1:A:23:HIS:HD2	2:A:528:HOH:O	1.99	0.45
1:A:422:PRO:HG2	1:A:425:ASP:HB2	1.98	0.45
1:B:6:ARG:NH2	1:B:68:ASP:OD1	2.47	0.45
1:A:301:ARG:HB3	2:A:747:HOH:O	2.16	0.44
1:A:107:LEU:HD11	1:B:195:PRO:HB2	1.99	0.44
1:B:411:ARG:HG3	2:B:566:HOH:O	2.17	0.44
1:A:444:ALA:O	1:A:445:ASP:C	2.55	0.44
1:A:288:ARG:HH21	1:A:291:HIS:CE1	2.34	0.44
1:A:398:GLY:O	1:A:399:HIS:HB2	2.16	0.44
1:A:33:LYS:HG2	1:A:117:ASP:C	2.38	0.44
1:B:178:GLU:HA	1:B:178:GLU:OE2	2.18	0.44
1:A:337:ARG:HG2	1:A:341:TYR:OH	2.17	0.44
1:A:159:LEU:HD22	1:A:380:PHE:HZ	1.83	0.44
1:A:424:LEU:O	1:A:428:ARG:HD2	2.18	0.44
1:A:168:LYS:HE2	1:A:168:LYS:HB2	1.56	0.44
1:B:310:LYS:N	2:B:738:HOH:O	2.50	0.44
1:B:136:PHE:O	2:B:613:HOH:O	2.21	0.44
1:A:217:ARG:HD2	1:A:217:ARG:HH11	1.70	0.44
1:A:147:TRP:CD2	1:A:157:GLY:HA3	2.53	0.44
1:B:65:ARG:HH12	1:B:88:ALA:N	2.10	0.44
1:B:424:LEU:CD1	1:B:437:PHE:CE2	3.01	0.44
1:B:51:THR:OG1	1:B:68:ASP:OD1	2.24	0.44
1:B:33:LYS:N	1:B:117:ASP:O	2.42	0.44
1:B:294:VAL:HG13	1:B:302:GLY:HA3	2.00	0.43
1:A:288:ARG:HH11	1:A:288:ARG:HD3	1.46	0.43
1:B:3:GLN:HB3	1:B:3:GLN:HE21	1.56	0.43
1:A:373:ALA:O	1:A:377:PRO:HD3	2.19	0.43
1:B:294:VAL:CG1	1:B:302:GLY:HA3	2.49	0.43
1:B:213:ASP:OD2	1:B:216:ARG:NH1	2.51	0.43
1:B:176:PHE:HE1	1:B:211:VAL:HG21	1.83	0.43
1:A:421:VAL:HG12	1:A:422:PRO:O	2.19	0.43
1:A:181:HIS:HB2	1:A:214:ALA:HB1	2.01	0.43
1:B:65:ARG:HH22	1:B:88:ALA:HB2	1.82	0.43
1:A:249:GLU:CD	2:A:721:HOH:O	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:HIS:CE1	1:B:65:ARG:HA	2.53	0.43
1:B:213:ASP:CB	2:B:702:HOH:O	2.67	0.43
1:A:424:LEU:HD11	1:A:451:TRP:CB	2.48	0.43
1:A:205:ARG:HA	1:A:246:TYR:CE2	2.54	0.43
1:A:86:PRO:HB2	1:A:89:LEU:HD13	2.00	0.42
1:A:219:GLN:HB2	2:A:487:HOH:O	2.18	0.42
1:B:361:LYS:HB2	1:B:361:LYS:HE3	1.59	0.42
1:B:265:TYR:HB3	1:B:289:ALA:O	2.18	0.42
1:B:374:LEU:HD11	1:B:437:PHE:HA	2.01	0.42
1:A:287:HIS:CD2	1:A:288:ARG:N	2.86	0.42
1:A:112:ASN:ND2	1:A:112:ASN:C	2.70	0.42
1:B:162:GLY:CA	1:B:189:PHE:O	2.67	0.42
1:A:290:GLY:C	1:A:292:GLY:N	2.67	0.42
1:B:336:ASP:C	1:B:338:ALA:H	2.21	0.42
1:A:434:ALA:HB1	2:A:776:HOH:O	2.19	0.42
1:A:3:GLN:C	1:A:5:SER:H	2.23	0.42
1:B:65:ARG:HH11	1:B:86:PRO:HB2	1.81	0.42
1:B:113:GLN:HE22	1:B:302:GLY:H	1.66	0.42
1:A:94:ILE:HD12	1:B:205:ARG:HH12	1.84	0.42
1:A:394:GLY:HA2	1:A:397:PHE:CD1	2.55	0.41
1:B:288:ARG:HB3	1:B:291:HIS:ND1	2.35	0.41
1:B:31:LYS:HG2	1:B:32:PRO:HD2	2.01	0.41
1:B:181:HIS:HB2	1:B:214:ALA:HB1	2.02	0.41
1:B:376:MET:HB3	1:B:377:PRO:CD	2.42	0.41
1:A:31:LYS:HA	1:A:32:PRO:HD3	1.90	0.41
1:A:374:LEU:HD11	1:A:437:PHE:HA	2.03	0.41
1:A:369:GLY:O	1:A:393:GLY:N	2.49	0.41
1:B:347:GLU:HG2	1:B:354:ARG:NH1	2.35	0.41
1:A:40:ALA:O	1:A:43:ALA:HB3	2.20	0.41
1:B:288:ARG:HH11	1:B:288:ARG:HD2	1.49	0.41
1:B:309:CYS:HB2	2:B:738:HOH:O	2.21	0.41
1:A:354:ARG:HB2	1:A:354:ARG:HE	1.44	0.41
1:B:415:GLN:HB2	1:B:415:GLN:HE21	1.44	0.41
1:A:452:ARG:CG	1:A:457:VAL:HG23	2.45	0.41
1:B:424:LEU:HD13	1:B:437:PHE:CE2	2.55	0.41
1:B:44:HIS:CD2	1:B:115:MET:HE2	2.56	0.41
1:B:278:ARG:NE	2:B:737:HOH:O	2.46	0.41
1:A:33:LYS:CG	1:A:117:ASP:C	2.89	0.40
1:A:400:ILE:HD11	1:A:435:ARG:CZ	2.51	0.40
1:A:337:ARG:HE	1:A:337:ARG:HB3	1.64	0.40
1:A:221:GLU:O	2:A:739:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASP:OD2	1:B:289:ALA:CB	2.49	0.40
1:B:65:ARG:CZ	1:B:88:ALA:H	2.31	0.40
1:A:65:ARG:HB3	1:A:66:GLY:H	1.38	0.40
1:B:231:ASN:HD21	1:B:233:THR:CB	2.35	0.40
1:B:371:MET:HE2	1:B:379:PHE:CG	2.56	0.40
1:A:30:MET:O	1:A:79:GLU:HB3	2.22	0.40

All (1) 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:359:GLY:O	1:A:431:LYS:NZ[2_646]	1.94	0.26

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	430/490 (88%)	404 (94%)	20 (5%)	6 (1%)	14 2
1	B	427/490 (87%)	404 (95%)	17 (4%)	6 (1%)	14 2
All	All	857/980 (87%)	808 (94%)	37 (4%)	12 (1%)	14 2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	B	3	GLN
1	B	112	ASN
1	A	33	LYS
1	A	34	ALA
1	A	52	GLY
1	A	335	SER

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Mol	Chain	Res	Type
1	B	292	GLY
1	B	456	GLY
1	A	5	SER
1	B	110	GLY
1	B	116	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	329/376 (88%)	302 (92%)	27 (8%)	14 3
1	B	326/376 (87%)	298 (91%)	28 (9%)	13 3
All	All	655/752 (87%)	600 (92%)	55 (8%)	14 3

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ARG
1	A	9	ASN
1	A	65	ARG
1	A	107	LEU
1	A	109	MET
1	A	112	ASN
1	A	130	GLU
1	A	141	VAL
1	A	166	LYS
1	A	194	GLU
1	A	222	THR
1	A	284	LEU
1	A	286	TYR
1	A	298	GLN
1	A	301	ARG
1	A	324	THR
1	A	336	ASP

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Mol	Chain	Res	Type
1	A	356	SER
1	A	371	MET
1	A	375	ARG
1	A	376	MET
1	A	424	LEU
1	A	431	LYS
1	A	443	ASP
1	A	446	GLN
1	A	453	LYS
1	B	3	GLN
1	B	5	SER
1	B	13	LYS
1	B	33	LYS
1	B	48	GLU
1	B	65	ARG
1	B	67	VAL
1	B	74	VAL
1	B	111	ASN
1	B	112	ASN
1	B	130	GLU
1	B	141	VAL
1	B	168	LYS
1	B	192	ASN
1	B	194	GLU
1	B	222	THR
1	B	284	LEU
1	B	286	TYR
1	B	298	GLN
1	B	301	ARG
1	B	347	GLU
1	B	376	MET
1	B	424	LEU
1	B	429	GLU
1	B	431	LYS
1	B	446	GLN
1	B	453	LYS
1	B	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN

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Mol	Chain	Res	Type
1	A	9	ASN
1	A	23	HIS
1	A	93	ASN
1	A	111	ASN
1	A	112	ASN
1	A	113	GLN
1	A	287	HIS
1	A	308	HIS
1	A	382	ASN
1	A	385	ASN
1	A	415	GLN
1	B	3	GLN
1	B	23	HIS
1	B	111	ASN
1	B	112	ASN
1	B	113	GLN
1	B	231	ASN
1	B	308	HIS
1	B	321	HIS
1	B	372	ASN
1	B	415	GLN
1	B	446	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.