Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:47 PM GMT

PDB ID	:	1CHM
Title	:	ENZYMATIC MECHANISM OF CREATINE AMIDINOHYDROLASE AS DEDUCED FROM CRYSTAL STRUCTURES
Authors	:	Hoeffken, H.W.; Knof, S.H.; Bartlett, P.A.; Huber, R.; Moellering, H.; Schumacher, G.
Deposited on	:	1993-07-19
Resolution	:	1.90 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:

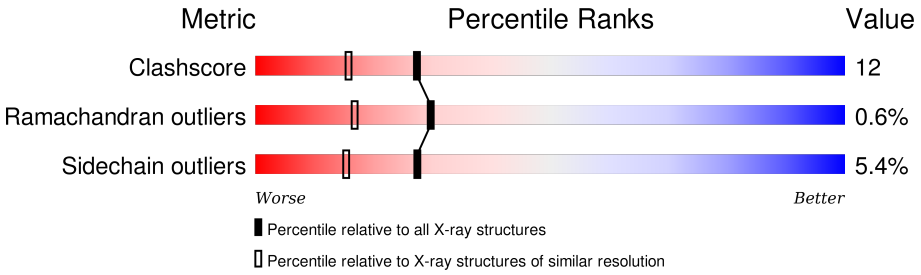
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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	401	51% 31% 15% •
1	B	401	56% 34% 7% •

2 Entry composition

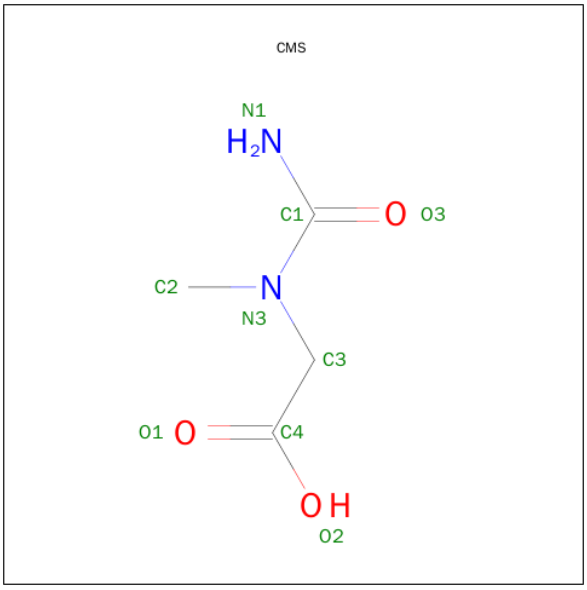
There are 3 unique types of molecules in this entry. The entry contains 6786 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CREATINE AMIDINOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	89	0	0
			3187	2004	568	598	17			
1	B	401	Total	C	N	O	S	96	0	0
			3187	2004	568	598	17			

- Molecule 2 is CARBAMOYL SARCOSINE (three-letter code: CMS) (formula: $C_4H_8N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	2	3		
2	B	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	198	Total O 198 198	0	0
3	B	196	Total O 196 196	0	0

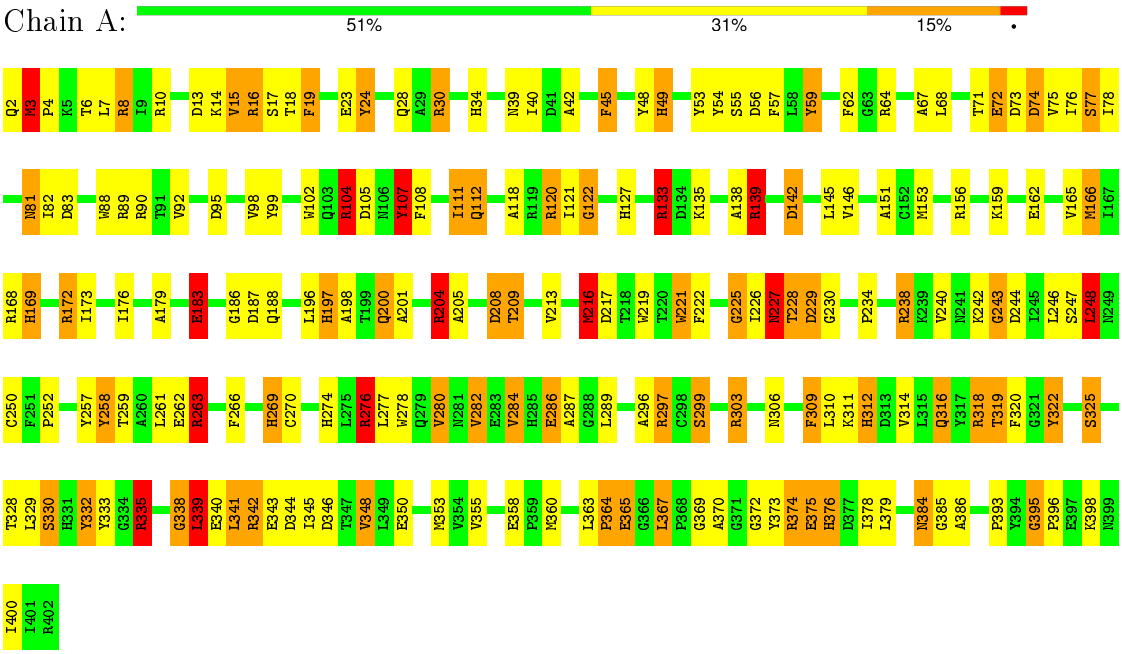
3 Residue-property plots (i)

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.

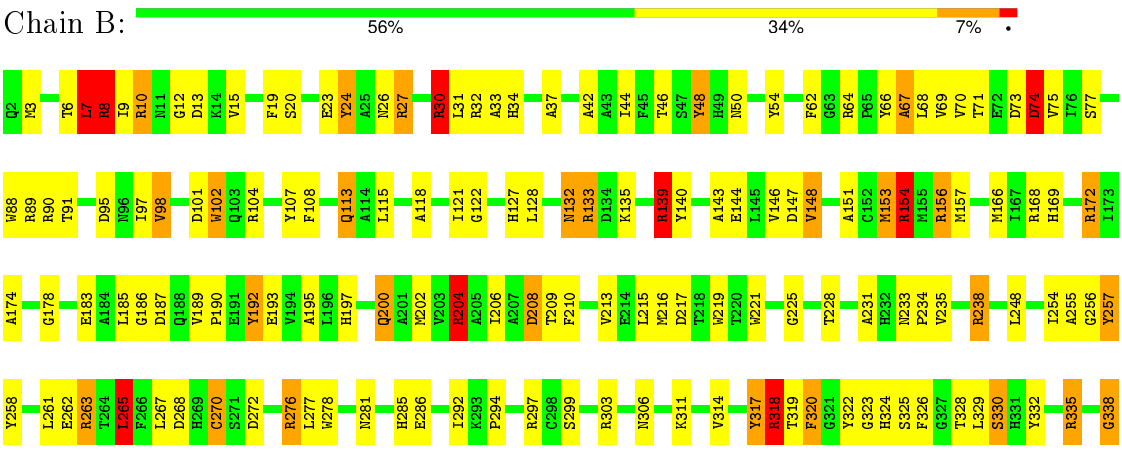
- Molecule 1: CREATINE AMIDINOHYDROLASE

Chain A:



- Molecule 1: CREATINE AMIDINOHYDROLASE

Chain B:




L339
R342
D346
V355
S356
M357
E358
L363
P364
E365
G366
L367
A370
G371
G372
Y373
R374
E375
H376
D377
I378
L379
N382
E383
A386
K391
F392
P393
N399
T400
T401
R402

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	60.83Å 110.55Å 62.63Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6786	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: CMS

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	1.76	48/3257 (1.5%)	2.62	122/4416 (2.8%)
1	B	1.72	36/3257 (1.1%)	2.37	115/4416 (2.6%)
All	All	1.74	84/6514 (1.3%)	2.50	237/8832 (2.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	6	69
1	B	5	44
All	All	11	113

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	GLU	CD-OE1	9.84	1.36	1.25
1	A	276	ARG	NE-CZ	9.07	1.44	1.33
1	A	263	ARG	NE-CZ	-8.96	1.21	1.33
1	A	365	GLU	CD-OE2	8.52	1.35	1.25
1	B	219	TRP	NE1-CE2	-8.00	1.27	1.37
1	A	219	TRP	NE1-CE2	-7.88	1.27	1.37
1	A	72	GLU	CB-CG	7.78	1.67	1.52
1	A	204	ARG	CZ-NH1	-7.74	1.23	1.33
1	B	89	ARG	CZ-NH2	7.69	1.43	1.33
1	A	59	TYR	CE2-CZ	7.65	1.48	1.38
1	B	197	HIS	CE1-NE2	7.51	1.50	1.32
1	A	221	TRP	NE1-CE2	-7.34	1.28	1.37
1	A	34	HIS	CE1-NE2	7.30	1.49	1.32
1	A	10	ARG	CZ-NH1	-7.29	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	ARG	CD-NE	-7.26	1.34	1.46
1	A	374	ARG	NE-CZ	7.21	1.42	1.33
1	B	278	TRP	NE1-CE2	-7.12	1.28	1.37
1	A	102	TRP	NE1-CE2	-7.11	1.28	1.37
1	B	318	ARG	CZ-NH2	7.00	1.42	1.33
1	B	32	ARG	CZ-NH1	-6.99	1.24	1.33
1	B	204	ARG	NE-CZ	6.96	1.42	1.33
1	B	3	MET	N-CA	6.91	1.60	1.46
1	B	221	TRP	NE1-CE2	-6.77	1.28	1.37
1	A	330	SER	CA-CB	6.75	1.63	1.52
1	B	178	GLY	N-CA	6.67	1.56	1.46
1	A	55	SER	CB-OG	6.62	1.50	1.42
1	B	373	TYR	CE2-CZ	6.57	1.47	1.38
1	B	139	ARG	CZ-NH1	6.54	1.41	1.33
1	B	219	TRP	CD1-NE1	6.52	1.49	1.38
1	A	303	ARG	NE-CZ	6.51	1.41	1.33
1	A	49	HIS	CE1-NE2	6.43	1.47	1.32
1	B	320	PHE	N-CA	6.42	1.59	1.46
1	B	324	HIS	ND1-CE1	6.38	1.50	1.34
1	B	66	TYR	CE2-CZ	6.35	1.46	1.38
1	A	276	ARG	CZ-NH1	6.35	1.41	1.33
1	A	64	ARG	NE-CZ	-6.21	1.25	1.33
1	A	243	GLY	N-CA	6.17	1.55	1.46
1	A	369	GLY	N-CA	6.17	1.55	1.46
1	A	340	GLU	CD-OE2	6.17	1.32	1.25
1	B	285	HIS	CE1-NE2	6.09	1.46	1.32
1	A	169	HIS	CE1-NE2	6.04	1.46	1.32
1	A	297	ARG	CZ-NH2	6.04	1.41	1.33
1	B	122	GLY	N-CA	6.03	1.55	1.46
1	B	66	TYR	CZ-OH	-6.00	1.27	1.37
1	B	15	VAL	C-N	5.91	1.47	1.34
1	A	54	TYR	CE2-CZ	5.90	1.46	1.38
1	A	287	ALA	C-N	5.89	1.43	1.33
1	B	297	ARG	CZ-NH2	5.84	1.40	1.33
1	A	111	ILE	N-CA	5.83	1.57	1.46
1	A	250	CYS	CB-SG	-5.82	1.72	1.81
1	B	377	ASP	C-N	5.79	1.47	1.34
1	A	198	ALA	C-N	-5.78	1.20	1.34
1	B	258	TYR	CE2-CZ	5.78	1.46	1.38
1	B	75	VAL	N-CA	5.77	1.57	1.46
1	A	88	TRP	NE1-CE2	-5.72	1.30	1.37
1	A	99	TYR	CE2-CZ	-5.66	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	TRP	NE1-CE2	-5.61	1.30	1.37
1	A	108	PHE	CE2-CZ	5.60	1.48	1.37
1	A	312	HIS	ND1-CE1	5.60	1.48	1.34
1	B	101	ASP	N-CA	5.58	1.57	1.46
1	A	333	TYR	CE1-CZ	5.57	1.45	1.38
1	B	258	TYR	CE1-CZ	5.55	1.45	1.38
1	B	127	HIS	CE1-NE2	5.49	1.45	1.32
1	A	276	ARG	CZ-NH2	5.48	1.40	1.33
1	B	8	ARG	NE-CZ	-5.46	1.25	1.33
1	B	20	SER	CB-OG	5.40	1.49	1.42
1	A	269	HIS	CG-ND1	5.36	1.50	1.38
1	B	197	HIS	CG-ND1	5.34	1.50	1.38
1	B	303	ARG	CD-NE	5.30	1.55	1.46
1	A	64	ARG	CD-NE	-5.29	1.37	1.46
1	A	274	HIS	ND1-CE1	5.28	1.48	1.34
1	A	252	PRO	N-CD	5.28	1.55	1.47
1	A	319	THR	CB-OG1	5.27	1.53	1.43
1	B	402	ARG	C-OXT	5.25	1.33	1.23
1	A	166	MET	N-CA	5.20	1.56	1.46
1	A	269	HIS	ND1-CE1	5.19	1.47	1.34
1	B	277	LEU	N-CA	5.16	1.56	1.46
1	B	88	TRP	CB-CG	5.12	1.59	1.50
1	A	204	ARG	NE-CZ	-5.11	1.26	1.33
1	B	233	ASN	CG-ND2	5.11	1.45	1.32
1	A	8	ARG	CZ-NH2	-5.08	1.26	1.33
1	A	90	ARG	CD-NE	5.03	1.54	1.46
1	A	200	GLN	CD-NE2	5.03	1.45	1.32
1	B	317	TYR	CE1-CZ	5.01	1.45	1.38

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	263	ARG	NE-CZ-NH2	-52.79	93.91	120.30
1	B	89	ARG	NE-CZ-NH1	-39.61	100.50	120.30
1	A	64	ARG	NE-CZ-NH1	-39.52	100.54	120.30
1	A	263	ARG	NE-CZ-NH1	38.24	139.42	120.30
1	A	204	ARG	NE-CZ-NH1	-36.95	101.82	120.30
1	A	64	ARG	NE-CZ-NH2	31.87	136.24	120.30
1	A	89	ARG	NE-CZ-NH1	-27.36	106.62	120.30
1	B	238	ARG	NE-CZ-NH2	26.29	133.44	120.30
1	B	89	ARG	NE-CZ-NH2	25.69	133.15	120.30
1	B	276	ARG	NE-CZ-NH1	24.55	132.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	238	ARG	NE-CZ-NH1	-24.01	108.30	120.30
1	A	168	ARG	NE-CZ-NH2	-22.06	109.27	120.30
1	A	200	GLN	CG-CD-OE1	-21.88	77.85	121.60
1	A	200	GLN	OE1-CD-NE2	20.72	169.56	121.90
1	B	89	ARG	CD-NE-CZ	19.89	151.44	123.60
1	B	263	ARG	NE-CZ-NH2	-19.58	110.51	120.30
1	B	263	ARG	NE-CZ-NH1	19.45	130.03	120.30
1	B	64	ARG	NE-CZ-NH2	-18.70	110.95	120.30
1	A	166	MET	CG-SD-CE	-16.58	73.67	100.20
1	B	27	ARG	NE-CZ-NH1	-16.27	112.16	120.30
1	A	318	ARG	NE-CZ-NH1	16.06	128.33	120.30
1	A	89	ARG	NE-CZ-NH2	15.28	127.94	120.30
1	B	335	ARG	NE-CZ-NH2	-15.25	112.68	120.30
1	B	30	ARG	NE-CZ-NH1	14.85	127.72	120.30
1	B	133	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	A	89	ARG	CD-NE-CZ	14.55	143.97	123.60
1	A	139	ARG	NE-CZ-NH2	-14.47	113.07	120.30
1	A	187	ASP	CB-CG-OD2	-14.45	105.29	118.30
1	B	30	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	A	10	ARG	NE-CZ-NH1	-13.49	113.56	120.30
1	B	133	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	64	ARG	CD-NE-CZ	13.35	142.29	123.60
1	A	8	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	B	263	ARG	CD-NE-CZ	12.28	140.80	123.60
1	B	342	ARG	NE-CZ-NH2	12.04	126.32	120.30
1	A	204	ARG	CD-NE-CZ	-11.66	107.28	123.60
1	A	30	ARG	CD-NE-CZ	-11.61	107.34	123.60
1	A	204	ARG	NE-CZ-NH2	11.40	126.00	120.30
1	A	8	ARG	NE-CZ-NH2	-11.33	114.64	120.30
1	A	30	ARG	NE-CZ-NH1	-11.31	114.64	120.30
1	B	373	TYR	CB-CG-CD1	-11.19	114.28	121.00
1	B	172	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	187	ASP	CB-CG-OD1	10.88	128.09	118.30
1	B	156	ARG	NE-CZ-NH1	-10.71	114.94	120.30
1	A	276	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	A	172	ARG	NE-CZ-NH2	10.59	125.60	120.30
1	A	30	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	200	GLN	CG-CD-NE2	-10.41	91.72	116.70
1	A	229	ASP	CB-CG-OD1	10.40	127.66	118.30
1	B	8	ARG	NE-CZ-NH1	-9.96	115.32	120.30
1	B	154	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	B	318	ARG	N-CA-CB	-9.70	93.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	187	ASP	CB-CG-OD1	9.61	126.95	118.30
1	A	374	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	B	187	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	A	344	ASP	CB-CG-OD1	8.75	126.18	118.30
1	B	216	MET	CA-C-N	-8.67	98.12	117.20
1	B	238	ARG	CD-NE-CZ	8.67	135.74	123.60
1	A	333	TYR	CB-CG-CD1	-8.67	115.80	121.00
1	B	32	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	104	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	B	146	VAL	CG1-CB-CG2	-8.43	97.41	110.90
1	A	216	MET	CG-SD-CE	8.40	113.64	100.20
1	A	258	TYR	CB-CG-CD2	-8.20	116.08	121.00
1	B	276	ARG	NH1-CZ-NH2	-8.08	110.51	119.40
1	A	45	PHE	CB-CG-CD1	-7.94	115.24	120.80
1	A	246	LEU	CB-CG-CD2	7.83	124.31	111.00
1	B	257	TYR	CB-CG-CD1	-7.82	116.31	121.00
1	B	335	ARG	NH1-CZ-NH2	7.75	127.92	119.40
1	B	258	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	B	204	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	90	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	259	THR	CA-CB-CG2	7.48	122.87	112.40
1	B	64	ARG	NH1-CZ-NH2	7.47	127.61	119.40
1	B	24	TYR	CB-CG-CD2	-7.40	116.56	121.00
1	A	168	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	89	ARG	CG-CD-NE	-7.29	96.48	111.80
1	A	83	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	153	MET	CG-SD-CE	-7.28	88.56	100.20
1	B	13	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	B	314	VAL	CA-CB-CG2	7.24	121.75	110.90
1	A	263	ARG	CD-NE-CZ	7.23	133.73	123.60
1	A	303	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	B	144	GLU	CA-CB-CG	-7.20	97.56	113.40
1	B	192	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	B	135	LYS	N-CA-CB	7.15	123.48	110.60
1	A	229	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	B	69	VAL	CG1-CB-CG2	7.07	122.20	110.90
1	B	154	ARG	CD-NE-CZ	7.05	133.48	123.60
1	B	208	ASP	CA-CB-CG	-7.05	97.89	113.40
1	B	8	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	120	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	342	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	3	MET	CA-CB-CG	-6.89	101.58	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	263	ARG	CB-CG-CD	6.84	129.39	111.60
1	B	276	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	172	ARG	NE-CZ-NH1	-6.81	116.90	120.30
1	B	373	TYR	CB-CG-CD2	6.79	125.07	121.00
1	B	317	TYR	CA-CB-CG	-6.78	100.51	113.40
1	A	318	ARG	NH1-CZ-NH2	-6.78	111.94	119.40
1	B	342	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	B	168	ARG	NE-CZ-NH1	-6.73	116.94	120.30
1	A	303	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	B	216	MET	O-C-N	6.72	133.46	122.70
1	A	240	VAL	CA-CB-CG1	6.71	120.97	110.90
1	A	342	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	B	67	ALA	N-CA-CB	6.69	119.47	110.10
1	B	270	CYS	N-CA-CB	-6.63	98.66	110.60
1	A	62	PHE	CB-CG-CD1	-6.63	116.16	120.80
1	A	168	ARG	NH1-CZ-NH2	6.62	126.69	119.40
1	A	53	TYR	CB-CG-CD2	-6.59	117.04	121.00
1	A	398	LYS	N-CA-CB	-6.59	98.73	110.60
1	B	383	GLU	CA-C-N	-6.58	102.73	117.20
1	B	166	MET	N-CA-CB	-6.47	98.95	110.60
1	B	332	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	A	263	ARG	NH1-CZ-NH2	6.40	126.44	119.40
1	B	147	ASP	C-N-CA	-6.39	105.72	121.70
1	B	27	ARG	NH1-CZ-NH2	6.39	126.43	119.40
1	B	187	ASP	O-C-N	6.37	132.89	122.70
1	A	108	PHE	O-C-N	6.37	132.89	122.70
1	A	276	ARG	CD-NE-CZ	6.35	132.49	123.60
1	B	89	ARG	CG-CD-NE	-6.31	98.55	111.80
1	A	238	ARG	CD-NE-CZ	6.28	132.39	123.60
1	B	118	ALA	N-CA-CB	6.24	118.84	110.10
1	B	102	TRP	CB-CA-C	-6.22	97.96	110.40
1	B	127	HIS	CA-CB-CG	-6.20	103.06	113.60
1	A	322	TYR	C-N-CA	-6.17	109.34	122.30
1	A	339	LEU	CB-CA-C	6.13	121.85	110.20
1	A	179	ALA	N-CA-CB	-6.12	101.53	110.10
1	B	216	MET	CB-CA-C	-6.12	98.17	110.40
1	A	365	GLU	CA-C-N	-6.08	104.03	116.20
1	B	154	ARG	CA-C-O	-6.08	107.33	120.10
1	B	386	ALA	CB-CA-C	-6.08	100.98	110.10
1	B	7	LEU	CB-CG-CD1	6.07	121.33	111.00
1	B	335	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	B	297	ARG	NE-CZ-NH1	-6.06	117.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	SER	N-CA-CB	-6.04	101.44	110.50
1	B	139	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	187	ASP	O-C-N	6.01	132.31	122.70
1	B	133	ARG	CG-CD-NE	-6.01	99.18	111.80
1	A	335	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	107	TYR	CB-CG-CD1	5.92	124.56	121.00
1	A	186	GLY	N-CA-C	-5.91	98.33	113.10
1	A	64	ARG	CG-CD-NE	-5.91	99.40	111.80
1	A	395	GLY	CA-C-O	5.88	131.19	120.60
1	A	365	GLU	CA-CB-CG	-5.85	100.53	113.40
1	A	8	ARG	CG-CD-NE	-5.84	99.53	111.80
1	B	338	GLY	C-N-CA	5.82	136.26	121.70
1	A	201	ALA	CB-CA-C	5.82	118.83	110.10
1	B	89	ARG	CB-CA-C	-5.81	98.78	110.40
1	A	127	HIS	CA-CB-CG	-5.80	103.74	113.60
1	A	3	MET	CA-C-N	5.80	133.33	117.10
1	B	317	TYR	C-N-CA	-5.79	107.22	121.70
1	A	15	VAL	CG1-CB-CG2	5.77	120.13	110.90
1	B	383	GLU	N-CA-CB	5.76	120.98	110.60
1	A	248	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	338	GLY	C-N-CA	5.75	136.07	121.70
1	A	107	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	B	325	SER	N-CA-CB	-5.72	101.92	110.50
1	B	255	ALA	N-CA-CB	5.71	118.10	110.10
1	B	204	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
1	A	133	ARG	CD-NE-CZ	5.68	131.56	123.60
1	A	303	ARG	CB-CG-CD	-5.68	96.84	111.60
1	A	384	ASN	CB-CA-C	-5.66	99.08	110.40
1	B	69	VAL	CA-CB-CG1	5.65	119.38	110.90
1	B	263	ARG	CB-CA-C	5.64	121.69	110.40
1	A	24	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	A	242	LYS	C-N-CA	-5.61	110.53	122.30
1	B	204	ARG	CB-CG-CD	-5.59	97.05	111.60
1	A	257	TYR	CA-CB-CG	-5.58	102.80	113.40
1	A	145	LEU	CB-CG-CD1	5.57	120.47	111.00
1	B	285	HIS	CA-CB-CG	-5.55	104.16	113.60
1	A	247	SER	N-CA-CB	-5.52	102.22	110.50
1	B	200	GLN	CB-CG-CD	-5.52	97.25	111.60
1	A	77	SER	O-C-N	-5.51	113.88	122.70
1	A	227	ASN	CB-CG-OD1	-5.49	110.63	121.60
1	A	350	GLU	CB-CA-C	-5.47	99.45	110.40
1	A	108	PHE	CB-CG-CD2	-5.47	116.97	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	286	GLU	CA-CB-CG	-5.47	101.37	113.40
1	A	138	ALA	N-CA-CB	-5.47	102.44	110.10
1	A	303	ARG	CD-NE-CZ	-5.46	115.96	123.60
1	A	367	LEU	CD1-CG-CD2	-5.45	94.14	110.50
1	B	132	ASN	N-CA-CB	5.45	120.41	110.60
1	B	297	ARG	CB-CG-CD	-5.43	97.48	111.60
1	B	377	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	376	HIS	CB-CA-C	-5.43	99.54	110.40
1	A	353	MET	CA-CB-CG	-5.43	104.08	113.30
1	B	208	ASP	CB-CG-OD1	-5.39	113.44	118.30
1	A	325	SER	N-CA-CB	-5.39	102.41	110.50
1	B	48	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	A	277	LEU	O-C-N	5.38	131.31	122.70
1	B	265	LEU	N-CA-CB	5.37	121.14	110.40
1	A	284	VAL	CA-CB-CG1	-5.37	102.84	110.90
1	A	332	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	299	SER	N-CA-CB	-5.36	102.46	110.50
1	A	104	ARG	CA-CB-CG	5.36	125.19	113.40
1	B	346	ASP	CA-CB-CG	-5.36	101.61	113.40
1	A	346	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	10	ARG	CG-CD-NE	-5.33	100.60	111.80
1	A	208	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	B	219	TRP	CD2-CE3-CZ3	-5.29	111.93	118.80
1	B	383	GLU	O-C-N	5.27	131.14	122.70
1	A	102	TRP	CB-CG-CD2	5.27	133.45	126.60
1	B	342	ARG	O-C-N	5.24	131.09	122.70
1	B	68	LEU	CB-CA-C	-5.24	100.25	110.20
1	A	165	VAL	CA-CB-CG2	-5.23	103.06	110.90
1	B	399	ASN	CB-CA-C	5.23	120.86	110.40
1	A	30	ARG	CA-CB-CG	-5.23	101.90	113.40
1	B	219	TRP	CE3-CZ3-CH2	5.22	126.94	121.20
1	A	328	THR	CA-CB-CG2	5.21	119.70	112.40
1	A	102	TRP	CH2-CZ2-CE2	-5.20	112.20	117.40
1	B	157	MET	CG-SD-CE	-5.19	91.89	100.20
1	B	311	LYS	C-N-CA	-5.19	108.72	121.70
1	A	363	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	A	209	THR	CA-CB-CG2	5.16	119.63	112.40
1	B	74	ASP	CB-CG-OD1	-5.16	113.65	118.30
1	A	3	MET	CA-C-O	-5.15	109.28	120.10
1	B	342	ARG	CD-NE-CZ	-5.15	116.39	123.60
1	A	18	THR	O-C-N	5.15	130.94	122.70
1	B	154	ARG	NH1-CZ-NH2	-5.15	113.74	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	238	ARG	CG-CD-NE	-5.15	100.99	111.80
1	B	67	ALA	CB-CA-C	5.13	117.80	110.10
1	A	297	ARG	N-CA-CB	5.12	119.81	110.60
1	B	209	THR	OG1-CB-CG2	-5.12	98.24	110.00
1	B	299	SER	N-CA-CB	-5.10	102.85	110.50
1	B	375	GLU	CG-CD-OE1	5.10	128.49	118.30
1	A	183	GLU	CB-CA-C	-5.08	100.23	110.40
1	B	330	SER	CA-CB-OG	-5.08	97.47	111.20
1	A	346	ASP	N-CA-C	5.08	124.73	111.00
1	B	318	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	393	PRO	O-C-N	5.08	130.82	122.70
1	A	39	ASN	CA-CB-CG	-5.07	102.25	113.40
1	A	133	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	386	ALA	N-CA-CB	-5.04	103.04	110.10
1	A	10	ARG	NH1-CZ-NH2	5.04	124.94	119.40
1	A	258	TYR	CB-CG-CD1	5.04	124.03	121.00
1	B	238	ARG	NH1-CZ-NH2	-5.02	113.88	119.40

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2	GLN	CA
1	A	71	THR	CB
1	A	104	ARG	CA
1	A	228	THR	CB
1	A	319	THR	CB
1	A	339	LEU	CA
1	B	71	THR	CB
1	B	228	THR	CB
1	B	319	THR	CB
1	B	339	LEU	CA
1	B	383	GLU	CA

All (113) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	A	107	TYR	Sidechain
1	A	112	GLN	Mainchain
1	A	118	ALA	Mainchain
1	A	122	GLY	Mainchain
1	A	13	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	133	ARG	Mainchain
1	A	139	ARG	Sidechain,Mainchain
1	A	14	LYS	Mainchain
1	A	142	ASP	Mainchain
1	A	151	ALA	Mainchain
1	A	156	ARG	Mainchain
1	A	159	LYS	Mainchain
1	A	16	ARG	Mainchain
1	A	162	GLU	Mainchain
1	A	17	SER	Mainchain
1	A	183	GLU	Mainchain
1	A	188	GLN	Mainchain
1	A	19	PHE	Mainchain
1	A	197	HIS	Mainchain
1	A	204	ARG	Sidechain,Mainchain
1	A	205	ALA	Mainchain
1	A	208	ASP	Mainchain
1	A	209	THR	Mainchain
1	A	216	MET	Mainchain
1	A	221	TRP	Mainchain
1	A	222	PHE	Mainchain
1	A	225	GLY	Mainchain
1	A	227	ASN	Sidechain,Mainchain
1	A	228	THR	Mainchain
1	A	230	GLY	Mainchain
1	A	234	PRO	Mainchain
1	A	263	ARG	Sidechain
1	A	266	PHE	Mainchain
1	A	270	CYS	Mainchain
1	A	28	GLN	Mainchain
1	A	280	VAL	Mainchain
1	A	282	VAL	Mainchain
1	A	286	GLU	Mainchain
1	A	296	ALA	Mainchain
1	A	30	ARG	Sidechain
1	A	303	ARG	Mainchain
1	A	310	LEU	Mainchain
1	A	311	LYS	Mainchain
1	A	312	HIS	Mainchain
1	A	330	SER	Mainchain
1	A	332	TYR	Mainchain
1	A	338	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	348	VAL	Mainchain
1	A	364	PRO	Mainchain
1	A	374	ARG	Sidechain
1	A	375	GLU	Mainchain
1	A	378	ILE	Mainchain
1	A	384	ASN	Mainchain
1	A	385	GLY	Mainchain
1	A	400	ILE	Mainchain
1	A	42	ALA	Mainchain
1	A	48	TYR	Mainchain
1	A	56	ASP	Mainchain
1	A	57	PHE	Mainchain
1	A	59	TYR	Mainchain
1	A	6	THR	Mainchain
1	A	74	ASP	Mainchain
1	A	77	SER	Mainchain
1	A	78	ILE	Mainchain
1	A	8	ARG	Sidechain
1	B	10	ARG	Sidechain
1	B	102	TRP	Mainchain
1	B	104	ARG	Mainchain
1	B	107	TYR	Sidechain
1	B	108	PHE	Mainchain
1	B	113	GLN	Mainchain
1	B	115	LEU	Mainchain
1	B	12	GLY	Mainchain
1	B	140	TYR	Mainchain
1	B	143	ALA	Mainchain
1	B	148	VAL	Mainchain
1	B	151	ALA	Mainchain
1	B	154	ARG	Mainchain
1	B	174	ALA	Mainchain
1	B	183	GLU	Mainchain
1	B	185	LEU	Mainchain
1	B	195	ALA	Mainchain
1	B	204	ARG	Mainchain
1	B	238	ARG	Sidechain
1	B	24	TYR	Sidechain
1	B	261	LEU	Mainchain
1	B	270	CYS	Mainchain
1	B	281	ASN	Mainchain
1	B	30	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	B	318	ARG	Sidechain
1	B	33	ALA	Mainchain
1	B	330	SER	Mainchain
1	B	338	GLY	Mainchain
1	B	356	SER	Mainchain
1	B	365	GLU	Mainchain
1	B	37	ALA	Mainchain
1	B	375	GLU	Mainchain
1	B	383	GLU	Peptide
1	B	400	ILE	Mainchain
1	B	42	ALA	Mainchain
1	B	48	TYR	Sidechain,Mainchain
1	B	54	TYR	Mainchain
1	B	67	ALA	Mainchain
1	B	74	ASP	Mainchain
1	B	77	SER	Mainchain
1	B	8	ARG	Sidechain
1	B	91	THR	Mainchain
1	B	98	VAL	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	3187	0	3097	72	0
1	B	3187	0	3096	74	0
2	A	9	0	7	1	0
2	B	9	0	7	2	0
3	A	198	0	0	3	0
3	B	196	0	0	5	0
All	All	6786	0	6207	145	0

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 12.

All (145) 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:263:ARG:HD3	1:A:393:PRO:O	1.81	0.80
1:B:71:THR:HG23	1:B:73:ASP:H	1.46	0.80
1:A:71:THR:HG23	1:A:73:ASP:H	1.46	0.80
1:A:225:GLY:O	1:A:228:THR:HG22	1.82	0.78
1:B:263:ARG:HD3	1:B:393:PRO:O	1.85	0.75
1:B:228:THR:HG23	1:B:372:GLY:H	1.52	0.74
1:B:265:LEU:HB2	1:B:401:ILE:HD11	1.70	0.74
1:A:196:LEU:O	1:A:200:GLN:HG3	1.89	0.73
1:B:265:LEU:N	1:B:265:LEU:HD23	2.07	0.70
1:B:225:GLY:O	1:B:228:THR:HG22	1.92	0.70
1:B:71:THR:HG23	1:B:74:ASP:H	1.58	0.68
1:B:363:LEU:HD23	1:B:367:LEU:HD23	1.73	0.68
1:A:339:LEU:HD11	1:A:355:VAL:HG11	1.75	0.67
1:A:76:ILE:HA	1:A:95:ASP:O	1.95	0.66
1:B:292:ILE:HD12	1:B:379:LEU:HD13	1.76	0.66
1:A:71:THR:CG2	1:A:74:ASP:H	2.07	0.66
1:A:226:ILE:HD12	1:A:365:GLU:HG3	1.77	0.65
1:A:227:ASN:ND2	1:A:238:ARG:HD3	2.12	0.65
1:B:262:GLU:HB2	1:B:376:HIS:HB3	1.78	0.65
1:A:358:GLU:HA	1:A:375:GLU:O	1.98	0.64
1:B:254:ILE:O	1:B:257:TYR:HB2	1.98	0.64
1:A:200:GLN:CD	1:B:200:GLN:HE21	2.02	0.63
1:B:19:PHE:HB3	1:B:23:GLU:HG2	1.80	0.63
1:A:183:GLU:OE1	1:A:197:HIS:HE1	1.80	0.63
1:B:319:THR:HG23	1:B:320:PHE:HD1	1.63	0.62
1:B:248:LEU:O	1:B:262:GLU:HA	2.00	0.62
1:B:71:THR:CG2	1:B:74:ASP:H	2.14	0.61
1:A:71:THR:HG23	1:A:74:ASP:H	1.67	0.60
1:B:228:THR:CG2	1:B:372:GLY:H	2.16	0.59
1:B:294:PRO:HG3	1:B:382:ASN:O	2.03	0.58
1:B:71:THR:HG22	1:B:74:ASP:HB2	1.84	0.58
1:A:319:THR:HG23	1:A:320:PHE:HD1	1.70	0.57
1:B:292:ILE:HD13	1:B:355:VAL:CG1	2.34	0.57
1:A:316:GLN:H	1:A:316:GLN:HE21	1.52	0.57
1:A:228:THR:CG2	1:A:372:GLY:H	2.18	0.56
1:A:200:GLN:O	1:A:204:ARG:HG3	2.06	0.56
2:B:404:CMS:C1	3:B:587:HOH:O	2.54	0.55
1:B:23:GLU:O	1:B:27:ARG:HG3	2.06	0.55
1:B:6:THR:HG21	1:B:113:GLN:HE22	1.71	0.54
1:B:263:ARG:HD2	1:B:392:PHE:HD2	1.73	0.54
1:B:71:THR:HG23	1:B:73:ASP:N	2.20	0.54
1:A:169:HIS:HD2	1:A:172:ARG:HH21	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:THR:CG2	1:B:97:ILE:HG23	2.38	0.53
1:A:49:HIS:HE1	3:A:502:HOH:O	1.91	0.53
1:B:265:LEU:HB2	1:B:401:ILE:CD1	2.37	0.53
1:B:200:GLN:HB3	1:B:204:ARG:HH21	1.73	0.53
1:B:210:PHE:HB2	1:B:213:VAL:HB	1.90	0.53
1:B:7:LEU:HD22	1:B:9:ILE:HD11	1.91	0.53
1:B:50:ASN:HD21	1:B:156:ARG:HH11	1.57	0.53
1:A:40:ILE:HG12	1:A:120:ARG:HD2	1.91	0.52
1:A:364:PRO:HD2	1:A:367:LEU:HD22	1.91	0.51
1:A:339:LEU:HD11	1:A:355:VAL:CG1	2.40	0.51
1:A:228:THR:HG23	1:A:372:GLY:H	1.74	0.51
1:B:263:ARG:HD2	1:B:392:PHE:CD2	2.45	0.51
1:B:6:THR:HG23	1:B:97:ILE:HG23	1.92	0.51
1:B:192:TYR:HA	1:B:235:VAL:HG11	1.92	0.50
1:B:186:GLY:O	1:B:189:VAL:HG12	2.11	0.50
1:A:3:MET:HB3	1:A:4:PRO:HD2	1.92	0.50
1:B:263:ARG:CD	1:B:392:PHE:HD2	2.25	0.50
1:B:272:ASP:O	1:B:276:ARG:HD3	2.11	0.50
1:A:282:VAL:O	1:A:286:GLU:HG3	2.12	0.49
1:B:6:THR:HG21	1:B:113:GLN:NE2	2.27	0.49
1:B:306:ASN:HD21	1:B:318:ARG:NH1	2.10	0.49
1:B:202:MET:O	1:B:206:ILE:HG13	2.12	0.49
1:A:19:PHE:HB3	1:A:23:GLU:HG2	1.93	0.49
1:B:292:ILE:HD13	1:B:355:VAL:HG11	1.95	0.48
1:A:216:MET:HG2	1:B:234:PRO:HB3	1.95	0.48
1:A:262:GLU:HB2	1:A:376:HIS:CB	2.44	0.48
1:B:363:LEU:HD23	1:B:367:LEU:CD2	2.41	0.48
1:A:297:ARG:HG2	1:A:348:VAL:HG22	1.96	0.48
1:B:262:GLU:HB2	1:B:376:HIS:CB	2.44	0.47
1:A:71:THR:HG23	1:A:73:ASP:N	2.23	0.47
1:B:401:ILE:H	1:B:401:ILE:HD12	1.79	0.47
1:A:173:ILE:O	1:A:176:ILE:HB	2.14	0.47
1:A:24:TYR:CB	1:A:92:VAL:HG11	2.45	0.47
1:A:262:GLU:HB2	1:A:376:HIS:HB2	1.97	0.47
1:B:169:HIS:CD2	1:B:172:ARG:HH21	2.33	0.47
1:B:26:ASN:O	1:B:30:ARG:HG3	2.14	0.47
1:B:6:THR:HA	1:B:98:VAL:O	2.15	0.47
1:A:343:GLU:N	1:A:343:GLU:OE1	2.47	0.47
1:B:256:GLY:O	1:B:328:THR:HA	2.15	0.46
1:A:228:THR:HG23	1:A:372:GLY:N	2.31	0.46
1:B:358:GLU:HA	1:B:375:GLU:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:OE1	1:A:197:HIS:CE1	2.65	0.46
1:B:7:LEU:CD2	1:B:9:ILE:HD11	2.45	0.46
1:A:71:THR:HG22	1:A:74:ASP:H	1.80	0.45
2:B:404:CMS:H23	3:B:587:HOH:O	2.15	0.45
1:A:82:ILE:HG12	1:B:231:ALA:HB3	1.97	0.45
1:B:326:PHE:CD1	1:B:326:PHE:N	2.84	0.45
1:A:306:ASN:HD21	1:A:318:ARG:HH11	1.62	0.45
1:B:7:LEU:N	1:B:7:LEU:HD12	2.31	0.45
1:B:306:ASN:ND2	1:B:322:TYR:OH	2.50	0.45
1:A:19:PHE:CB	1:A:23:GLU:HG2	2.46	0.45
1:A:306:ASN:HD21	1:A:318:ARG:NH1	2.15	0.45
1:A:135:LYS:O	1:A:139:ARG:HG2	2.16	0.45
1:B:6:THR:HG23	1:B:97:ILE:CG2	2.46	0.45
1:A:316:GLN:H	1:A:316:GLN:NE2	2.15	0.45
1:A:121:ILE:HD13	1:A:121:ILE:HG21	1.78	0.45
1:B:139:ARG:HH11	1:B:139:ARG:HD3	1.65	0.45
1:B:292:ILE:HD13	1:B:355:VAL:HG13	1.99	0.45
1:A:370:ALA:HB3	3:A:448:HOH:O	2.16	0.45
1:A:45:PHE:O	1:A:67:ALA:HA	2.16	0.45
1:A:258:TYR:HB2	1:A:329:LEU:O	2.16	0.45
1:A:112:GLN:HE21	1:A:139:ARG:HH11	1.66	0.44
1:A:107:TYR:CZ	1:A:111:ILE:HD11	2.53	0.44
1:B:367:LEU:O	1:B:370:ALA:HB2	2.17	0.44
1:A:81:ASN:HA	1:A:98:VAL:CG1	2.47	0.44
1:B:31:LEU:HD23	1:B:70:VAL:HG11	1.99	0.44
1:A:243:GLY:HA2	1:A:269:HIS:O	2.18	0.44
1:A:322:TYR:HB2	1:A:341:LEU:HB3	2.00	0.44
1:A:276:ARG:O	1:A:280:VAL:HG23	2.17	0.44
1:A:226:ILE:HG12	1:A:226:ILE:O	2.18	0.44
1:B:7:LEU:HD13	1:B:98:VAL:HB	1.99	0.43
1:B:31:LEU:O	1:B:34:HIS:HB3	2.18	0.43
1:B:267:LEU:HB3	3:B:542:HOH:O	2.18	0.43
1:A:395:GLY:HA2	1:A:396:PRO:HD3	1.75	0.43
1:A:104:ARG:HD2	1:A:105:ASP:OD1	2.19	0.43
1:B:319:THR:HG21	3:B:468:HOH:O	2.19	0.43
1:A:360:MET:HA	1:A:373:TYR:O	2.19	0.43
1:A:122:GLY:HA2	1:A:146:VAL:O	2.19	0.42
1:A:40:ILE:CG1	1:A:120:ARG:HD2	2.50	0.42
1:A:325:SER:HB2	1:A:339:LEU:HG	2.02	0.42
1:B:169:HIS:HD2	1:B:172:ARG:HH21	1.67	0.42
1:A:139:ARG:HD3	1:A:139:ARG:HA	1.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD11	1:A:75:VAL:HG12	2.01	0.42
1:B:323:GLY:HA3	1:B:356:SER:O	2.20	0.42
1:A:342:ARG:HB2	1:A:345:ILE:HG13	2.01	0.42
1:B:317:TYR:HA	1:B:317:TYR:HD1	1.63	0.41
1:B:190:PRO:HG2	1:B:193:GLU:HG2	2.02	0.41
1:A:71:THR:HG22	1:A:74:ASP:HB2	2.01	0.41
1:A:360:MET:HG3	1:A:373:TYR:O	2.20	0.41
1:A:169:HIS:CE1	3:A:546:HOH:O	2.73	0.41
1:B:44:ILE:HD12	1:B:121:ILE:HG21	2.03	0.41
1:B:210:PHE:CB	1:B:213:VAL:HB	2.49	0.41
1:B:8:ARG:NH1	1:B:95:ASP:OD2	2.54	0.41
1:B:215:LEU:HA	3:B:537:HOH:O	2.20	0.41
1:A:248:LEU:HD21	1:A:261:LEU:HD23	2.03	0.41
1:A:284:VAL:HG21	1:A:309:PHE:CE1	2.56	0.41
1:B:132:ASN:HD22	1:B:132:ASN:HA	1.49	0.41
1:B:262:GLU:CB	1:B:376:HIS:HB3	2.50	0.40
1:A:319:THR:HG21	1:A:360:MET:SD	2.61	0.40
1:A:335:ARG:HH12	2:A:404:CMS:C4	2.34	0.40
1:A:238:ARG:NH2	1:A:244:ASP:OD2	2.54	0.40
1:B:46:THR:HG21	1:B:128:LEU:HD13	2.03	0.40
1:A:289:LEU:HD22	1:A:379:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

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	399/401 (100%)	377 (94%)	19 (5%)	3 (1%)	24	11
1	B	399/401 (100%)	377 (94%)	20 (5%)	2 (0%)	34	21
All	All	798/802 (100%)	754 (94%)	39 (5%)	5 (1%)	30	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	ASP
1	A	3	MET
1	A	217	ASP
1	A	335	ARG
1	B	335	ARG

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	333/333 (100%)	311 (93%)	22 (7%)	21 10
1	B	333/333 (100%)	319 (96%)	14 (4%)	36 24
All	All	666/666 (100%)	630 (95%)	36 (5%)	27 15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	7	LEU
1	A	15	VAL
1	A	16	ARG
1	A	72	GLU
1	A	81	ASN
1	A	104	ARG
1	A	133	ARG
1	A	142	ASP
1	A	153	MET
1	A	166	MET
1	A	213	VAL
1	A	229	ASP
1	A	248	LEU
1	A	263	ARG
1	A	276	ARG
1	A	299	SER
1	A	309	PHE

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Mol	Chain	Res	Type
1	A	314	VAL
1	A	316	GLN
1	A	339	LEU
1	A	341	LEU
1	B	7	LEU
1	B	62	PHE
1	B	133	ARG
1	B	139	ARG
1	B	148	VAL
1	B	153	MET
1	B	154	ARG
1	B	204	ARG
1	B	208	ASP
1	B	265	LEU
1	B	268	ASP
1	B	329	LEU
1	B	339	LEU
1	B	391	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	26	ASN
1	A	49	HIS
1	A	50	ASN
1	A	112	GLN
1	A	132	ASN
1	A	169	HIS
1	A	197	HIS
1	A	306	ASN
1	A	316	GLN
1	B	26	ASN
1	B	49	HIS
1	B	50	ASN
1	B	81	ASN
1	B	113	GLN
1	B	132	ASN
1	B	169	HIS
1	B	197	HIS
1	B	200	GLN
1	B	306	ASN

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	CMS	A	404	-	4,8,8	0.83	0	3,10,10	4.36	3 (100%)
2	CMS	B	404	-	4,8,8	1.61	1 (25%)	3,10,10	1.73	1 (33%)

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	CMS	A	404	-	-	0/6/8/8	0/0/0/0
2	CMS	B	404	-	-	1/6/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	404	CMS	C1-N1	2.90	1.38	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	404	CMS	O3-C1-N1	-5.64	112.97	122.88
2	A	404	CMS	C2-N3-C3	-3.58	98.65	116.43
2	B	404	CMS	C2-N3-C3	-2.35	104.76	116.43
2	A	404	CMS	C4-C3-N3	3.52	121.43	113.84

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	404	CMS	N1-C1-N3-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	CMS	1	0
2	B	404	CMS	2	0

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.