



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:04 am GMT

PDB ID : 1FUG
Title : S-ADENOSYLMETHIONINE SYNTHETASE
Authors : Fu, Z.; Markham, G.D.; Takusagawa, F.
Deposited on : 1996-02-25
Resolution : 3.20 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

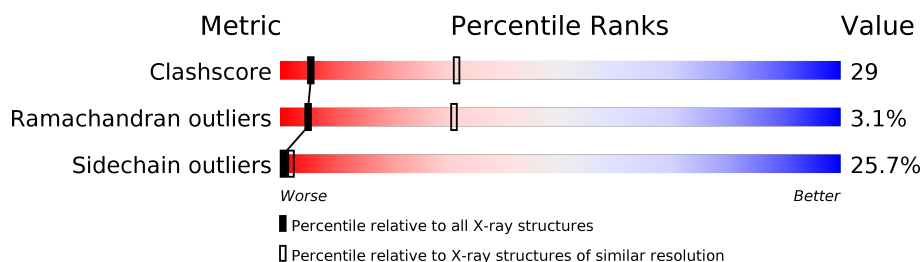
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)

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 $\leq 5\%$. 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	383	
1	B	383	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7170 atoms, of which 1286 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 S-ADENOSYLMETHIONINE SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	H	N	O	S	0	0	0
			3585	1856	643	503	570	13			
1	B	383	Total	C	H	N	O	S	0	0	0
			3585	1856	643	503	570	13			

3 Residue-property plots

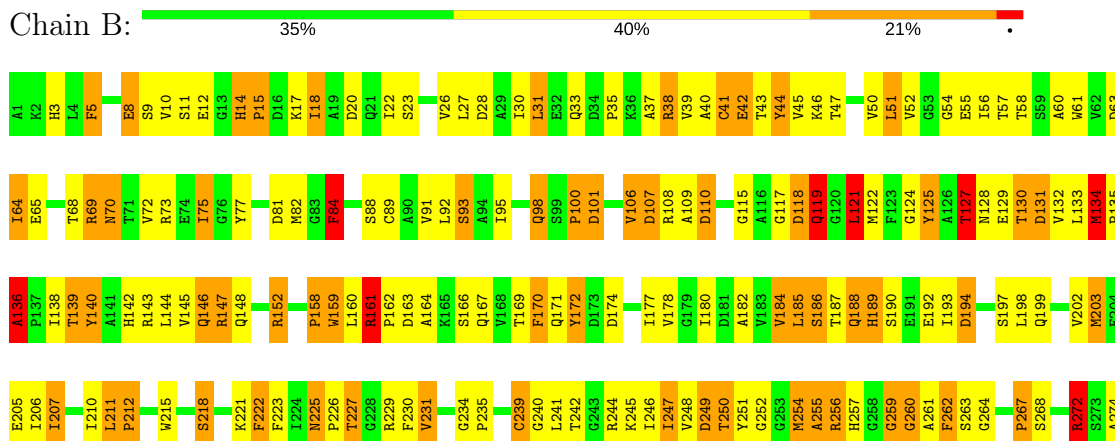
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: S-ADENOSYLMETHIONINE SYNTHETASE



• Molecule 1: S-ADENOSYLMETHIONINE SYNTHETASE



A275	A276	A277	A278	A279	A280	A281	A282	A283	A284	A285	A286	A287	A288	A289	A290	A291	A292	A293	A294	A295	A296	A297	A298	A299	A300	A301	A302	A303	A304	A305	A306	A307	A308	A309	A310	A311	A312	A313	A314	A315	A316	A317	A318	A319	A320	A321	A322	A323	A324	A325	A326	A327	A328	A329	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341																																	
Q342	M343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.00Å 121.00Å 171.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.4 (8.00-3.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.210 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	0.95	0/3001	1.93	76/4068 (1.9%)
1	B	0.92	1/3001 (0.0%)	1.97	79/4068 (1.9%)
All	All	0.94	1/6002 (0.0%)	1.95	155/8136 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	B	0	18
All	All	0	37

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	260	GLY	CA-C	5.17	1.60	1.51

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	B	279	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	A	244	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	A	244	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	B	272	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	B	377	ARG	NE-CZ-NH1	10.25	125.42	120.30
1	A	279	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	B	330	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	B	82	MET	CA-CB-CG	9.66	129.72	113.30
1	B	152	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	B	351	TYR	CB-CG-CD1	-9.30	115.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	A	61	TRP	CD1-CG-CD2	8.88	113.41	106.30
1	B	367	TRP	CD1-CG-CD2	8.67	113.24	106.30
1	A	239	CYS	CA-CB-SG	-8.62	98.48	114.00
1	B	259	GLY	CA-C-N	8.62	133.44	116.20
1	A	215	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	B	326	THR	CA-CB-CG2	8.46	124.24	112.40
1	A	61	TRP	CB-CG-CD1	-8.42	116.06	127.00
1	B	250	THR	CA-C-N	8.34	135.56	117.20
1	A	280	TYR	CB-CG-CD2	-8.25	116.05	121.00
1	A	236	MET	CG-SD-CE	-8.23	87.02	100.20
1	A	351	TYR	CB-CG-CD1	-8.07	116.16	121.00
1	A	61	TRP	CE2-CD2-CG	-8.03	100.87	107.30
1	B	101	ASP	CA-C-N	8.02	134.85	117.20
1	A	61	TRP	CG-CD2-CE3	7.98	141.08	133.90
1	B	261	ALA	O-C-N	7.91	135.36	122.70
1	B	159	TRP	CB-CG-CD1	-7.86	116.79	127.00
1	B	261	ALA	CA-C-N	-7.81	100.02	117.20
1	A	168	VAL	CG1-CB-CG2	-7.79	98.43	110.90
1	A	336	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	159	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	A	134	MET	CG-SD-CE	-7.60	88.03	100.20
1	A	255	ALA	CB-CA-C	-7.48	98.88	110.10
1	B	367	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	B	159	TRP	CG-CD2-CE3	7.38	140.54	133.90
1	A	7	SER	CA-CB-OG	-7.36	91.32	111.20
1	B	159	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	B	375	LEU	CA-CB-CG	7.25	131.98	115.30
1	B	215	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	A	26	VAL	CG1-CB-CG2	-7.11	99.53	110.90
1	A	10	VAL	CA-CB-CG2	-7.09	100.27	110.90
1	B	147	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	382	LEU	CA-CB-CG	6.95	131.28	115.30
1	B	215	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	B	108	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	100	PRO	N-CA-C	6.83	129.85	112.10
1	A	215	TRP	CE2-CD2-CG	-6.81	101.86	107.30
1	B	338	TYR	CB-CG-CD1	-6.74	116.96	121.00
1	A	152	ARG	CA-CB-CG	6.74	128.22	113.40
1	A	159	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	B	84	PHE	CB-CG-CD1	6.73	125.51	120.80
1	A	152	ARG	NE-CZ-NH2	-6.68	116.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	GLN	CA-CB-CG	6.64	128.02	113.40
1	B	61	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	B	61	TRP	CD1-CG-CD2	6.47	111.48	106.30
1	B	249	ASP	CA-CB-CG	6.38	127.44	113.40
1	A	293	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	60	ALA	CB-CA-C	-6.30	100.65	110.10
1	B	260	GLY	N-CA-C	6.30	128.84	113.10
1	A	159	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	B	69	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	227	THR	CA-C-N	-6.26	103.68	116.20
1	B	364	HIS	N-CA-CB	6.25	121.86	110.60
1	A	67	ILE	CG1-CB-CG2	-6.24	97.68	111.40
1	A	37	ALA	CB-CA-C	-6.20	100.80	110.10
1	B	314	THR	N-CA-C	-6.20	94.27	111.00
1	A	259	GLY	CA-C-N	6.13	128.46	116.20
1	B	256	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	215	TRP	CG-CD1-NE1	-6.12	103.98	110.10
1	A	272	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	78	VAL	O-C-N	-6.07	112.99	122.70
1	A	198	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	125	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	A	271	ASP	CB-CA-C	-5.99	98.43	110.40
1	B	152	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	146	GLN	CA-CB-CG	-5.95	100.32	113.40
1	B	326	THR	CA-CB-OG1	-5.93	96.54	109.00
1	A	61	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	B	367	TRP	CG-CD2-CE3	5.92	139.23	133.90
1	B	167	GLN	CB-CA-C	-5.92	98.57	110.40
1	B	367	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	B	250	THR	O-C-N	-5.90	113.26	122.70
1	B	259	GLY	C-N-CA	-5.89	109.92	122.30
1	A	262	PHE	CB-CG-CD2	-5.89	116.68	120.80
1	B	167	GLN	N-CA-CB	5.81	121.06	110.60
1	A	367	TRP	CE2-CD2-CG	-5.81	102.66	107.30
1	B	383	LYS	N-CA-C	5.80	126.65	111.00
1	A	215	TRP	CB-CG-CD1	-5.78	119.49	127.00
1	B	8	GLU	CA-CB-CG	5.77	126.09	113.40
1	A	269	LYS	N-CA-C	-5.76	95.45	111.00
1	A	217	THR	CA-CB-CG2	5.74	120.44	112.40
1	B	212	PRO	CA-C-N	-5.70	104.66	117.20
1	B	136	ALA	N-CA-C	5.64	126.24	111.00
1	B	51	LEU	CA-CB-CG	5.64	128.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	152	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	314	THR	N-CA-C	-5.63	95.80	111.00
1	B	121	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	334	ASP	CA-C-N	-5.60	104.87	117.20
1	A	290	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	128	ASN	N-CA-CB	5.56	120.61	110.60
1	B	134	MET	CG-SD-CE	-5.56	91.30	100.20
1	A	306	GLU	CB-CA-C	5.54	121.49	110.40
1	A	338	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	B	186	SER	N-CA-CB	5.52	118.78	110.50
1	B	239	CYS	CA-CB-SG	-5.52	104.07	114.00
1	A	1	ALA	N-CA-C	-5.51	96.13	111.00
1	A	133	LEU	N-CA-CB	-5.50	99.41	110.40
1	A	223	PHE	CB-CG-CD2	-5.49	116.96	120.80
1	A	377	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	101	ASP	O-C-N	-5.47	113.95	122.70
1	B	61	TRP	N-CA-C	-5.47	96.24	111.00
1	A	143	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	351	TYR	CA-C-N	5.45	129.19	117.20
1	A	69	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	360	PHE	N-CA-C	-5.43	96.34	111.00
1	A	202	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	A	367	TRP	CD1-CG-CD2	5.41	110.63	106.30
1	A	236	MET	CA-CB-CG	5.41	122.49	113.30
1	A	263	SER	CB-CA-C	-5.39	99.86	110.10
1	A	357	TYR	CA-CB-CG	-5.39	103.16	113.40
1	B	125	TYR	CB-CG-CD2	-5.38	117.78	121.00
1	B	44	TYR	N-CA-C	-5.36	96.52	111.00
1	B	255	ALA	CB-CA-C	-5.35	102.08	110.10
1	A	315	PHE	CA-C-N	-5.34	105.52	116.20
1	B	259	GLY	CA-C-O	-5.34	110.99	120.60
1	B	84	PHE	CA-CB-CG	5.33	126.70	113.90
1	A	50	VAL	N-CA-C	-5.33	96.60	111.00
1	A	176	LYS	CA-C-N	-5.32	105.49	117.20
1	B	146	GLN	N-CA-C	-5.30	96.69	111.00
1	B	14	HIS	CA-CB-CG	5.23	122.49	113.60
1	A	215	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	A	362	ARG	N-CA-C	-5.21	96.92	111.00
1	B	20	ASP	N-CA-CB	-5.20	101.24	110.60
1	A	133	LEU	CB-CA-C	5.19	120.06	110.20
1	A	4	LEU	CA-CB-CG	5.17	127.20	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	THR	CA-C-N	5.15	128.53	117.20
1	B	267	PRO	N-CD-CG	-5.15	95.47	103.20
1	A	311	MET	CA-CB-CG	5.15	122.05	113.30
1	A	256	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	377	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	185	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	B	336	ARG	CB-CG-CD	5.12	124.92	111.60
1	B	260	GLY	CA-C-O	5.11	129.79	120.60
1	A	232	ILE	N-CA-C	-5.10	97.24	111.00
1	B	250	THR	N-CA-C	5.10	124.77	111.00
1	A	108	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	279	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	42	GLU	CB-CA-C	-5.05	100.30	110.40
1	B	311	MET	CA-CB-CG	5.05	121.89	113.30
1	B	88	SER	N-CA-CB	-5.05	102.93	110.50
1	A	102	ILE	O-C-N	-5.05	114.63	122.70
1	B	229	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	102	ILE	CA-C-N	5.01	128.22	117.20

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ASP	Peptide
1	A	125	TYR	Sidechain
1	A	132	VAL	Mainchain
1	A	143	ARG	Sidechain
1	A	152	ARG	Mainchain
1	A	170	PHE	Sidechain
1	A	251	TYR	Sidechain
1	A	256	ARG	Sidechain
1	A	276	TYR	Sidechain
1	A	280	TYR	Sidechain
1	A	300	TYR	Sidechain
1	A	315	PHE	Sidechain
1	A	351	TYR	Sidechain
1	A	357	TYR	Sidechain
1	A	360	PHE	Sidechain
1	A	362	ARG	Sidechain
1	A	44	TYR	Sidechain
1	A	69	ARG	Sidechain
1	A	84	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	B	106	VAL	Peptide
1	B	107	ASP	Peptide
1	B	140	TYR	Sidechain
1	B	170	PHE	Peptide
1	B	172	TYR	Sidechain
1	B	260	GLY	Peptide
1	B	272	ARG	Sidechain
1	B	276	TYR	Sidechain
1	B	280	TYR	Sidechain
1	B	294	CYS	Peptide
1	B	300	TYR	Sidechain
1	B	315	PHE	Sidechain
1	B	336	ARG	Sidechain
1	B	338	TYR	Sidechain
1	B	359	HIS	Sidechain
1	B	363	GLU	Mainchain
1	B	38	ARG	Sidechain
1	B	84	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2942	643	2908	168	0
1	B	2942	643	2908	182	0
All	All	5884	1286	5816	336	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 29.

All (336) 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:B:45:VAL:HG12	1:B:50:VAL:HG13	1.54	0.87
1:A:30:ILE:HG12	1:A:58:THR:HG21	1.59	0.85
1:B:251:TYR:HB2	1:B:255:ALA:HB2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:MET:SD	1:B:222:PHE:HE2	2.01	0.83
1:B:134:MET:SD	1:B:279:ARG:NH2	2.51	0.83
1:B:276:TYR:HE1	1:B:359:HIS:HB3	1.45	0.81
1:B:152:ARG:HB3	1:B:160:LEU:HD11	1.64	0.80
1:B:45:VAL:HG22	1:B:240:GLY:HA3	1.64	0.80
1:A:121:LEU:HB2	1:A:297:GLN:HE22	1.47	0.79
1:A:134:MET:SD	1:A:279:ARG:NH2	2.55	0.79
1:A:15:PRO:HB2	1:A:240:GLY:HA3	1.64	0.78
1:A:177:ILE:HG13	1:A:215:TRP:CZ2	2.21	0.76
1:B:65:GLU:HG3	1:B:91:VAL:HG11	1.67	0.76
1:B:278:ALA:HA	1:B:281:VAL:HG23	1.69	0.75
1:B:134:MET:HG3	1:B:135:PRO:HD2	1.66	0.75
1:B:138:ILE:HB	1:B:252:GLY:HA2	1.69	0.74
1:A:292:ASP:HB2	1:A:317:THR:HG22	1.67	0.74
1:B:203:MET:SD	1:B:222:PHE:CE2	2.81	0.72
1:B:130:THR:OG1	1:B:136:ALA:HB3	1.93	0.69
1:A:21:GLN:HE21	1:A:352:LYS:HE3	1.56	0.68
1:B:72:VAL:HG11	1:B:84:PHE:CE1	2.28	0.68
1:A:281:VAL:HG21	1:A:296:ILE:HD12	1.76	0.68
1:A:266:ASP:HB2	1:A:267:PRO:HD2	1.74	0.68
1:A:157:LEU:HD23	1:A:159:TRP:CZ2	2.30	0.67
1:B:11:SER:HA	1:B:357:TYR:HE1	1.60	0.66
1:B:134:MET:HA	1:B:279:ARG:HH22	1.60	0.66
1:B:5:PHE:CE2	1:B:254:MET:SD	2.88	0.66
1:A:161:ARG:O	1:A:188:GLN:HB3	1.96	0.66
1:B:122:MET:HG2	1:B:274:ALA:HB3	1.78	0.66
1:A:157:LEU:HD22	1:A:160:LEU:HD21	1.78	0.66
1:A:203:MET:SD	1:A:222:PHE:CD2	2.89	0.65
1:A:46:LYS:HB3	1:A:239:CYS:SG	2.37	0.65
1:B:138:ILE:HB	1:B:252:GLY:CA	2.27	0.65
1:A:9:SER:HB2	1:A:141:ALA:HB1	1.78	0.65
1:A:10:VAL:HG23	1:A:165:LYS:HA	1.79	0.65
1:B:129:GLU:HG2	1:B:135:PRO:HA	1.78	0.65
1:B:147:ARG:HD3	1:B:206:ILE:HA	1.78	0.64
1:A:261:ALA:HB3	1:A:265:LYS:NZ	2.13	0.64
1:A:297:GLN:HB3	1:A:311:MET:HB3	1.80	0.64
1:B:50:VAL:HG23	1:B:89:CYS:SG	2.37	0.64
1:A:30:ILE:HG21	1:A:39:VAL:HG11	1.79	0.64
1:A:262:PHE:O	1:A:272:ARG:HD3	1.99	0.63
1:B:145:VAL:HG12	1:B:206:ILE:HD11	1.80	0.63
1:A:245:LYS:HA	1:A:245:LYS:HE3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:TYR:O	1:B:354:THR:HG22	1.99	0.62
1:B:11:SER:HB3	1:B:164:ALA:HB3	1.81	0.62
1:B:109:ALA:HB2	1:B:115:GLY:HA2	1.82	0.62
1:B:134:MET:SD	1:B:279:ARG:CZ	2.87	0.62
1:B:42:GLU:HA	1:B:242:THR:HG21	1.82	0.62
1:A:83:GLY:HA3	1:A:236:MET:HB2	1.80	0.62
1:B:72:VAL:HG11	1:B:84:PHE:HE1	1.65	0.62
1:A:37:ALA:CB	1:A:58:THR:HG22	2.30	0.62
1:B:357:TYR:H	1:B:362:ARG:NH2	1.97	0.61
1:A:172:TYR:HE1	1:A:177:ILE:HG22	1.65	0.61
1:A:12:GLU:HB2	1:A:21:GLN:OE1	2.01	0.61
1:A:52:VAL:HG11	1:A:64:ILE:HG21	1.83	0.61
1:B:298:VAL:HG13	1:B:310:ILE:HG22	1.83	0.61
1:A:314:THR:HB	1:A:317:THR:OG1	2.01	0.60
1:A:167:GLN:NE2	1:B:119:GLN:HG2	2.17	0.60
1:B:15:PRO:HA	1:B:18:ILE:HG22	1.82	0.60
1:A:30:ILE:CG2	1:A:39:VAL:HG11	2.32	0.60
1:A:37:ALA:HB2	1:A:58:THR:HG22	1.83	0.60
1:A:281:VAL:CG2	1:A:296:ILE:HD12	2.32	0.59
1:B:65:GLU:HA	1:B:91:VAL:HG21	1.83	0.59
1:A:9:SER:OG	1:A:142:HIS:HD2	1.86	0.59
1:A:263:SER:HA	1:A:272:ARG:NH1	2.18	0.59
1:A:320:VAL:HB	1:A:321:PRO:HD2	1.83	0.59
1:A:247:ILE:HB	1:B:259:GLY:CA	2.33	0.59
1:B:184:VAL:HB	1:B:223:PHE:HB2	1.84	0.59
1:B:295:GLU:HG2	1:B:315:PHE:HE1	1.68	0.59
1:A:46:LYS:HB3	1:A:239:CYS:HG	1.67	0.59
1:B:319:LYS:N	1:B:319:LYS:HD2	2.18	0.59
1:B:185:LEU:HD21	1:B:206:ILE:HD13	1.84	0.58
1:A:272:ARG:HG2	1:A:276:TYR:CE2	2.38	0.58
1:A:256:ARG:HH12	1:B:256:ARG:HH22	1.51	0.58
1:B:23:SER:CB	1:B:41:CYS:SG	2.92	0.58
1:A:122:MET:N	1:A:122:MET:SD	2.77	0.57
1:A:239:CYS:SG	1:A:240:GLY:N	2.76	0.57
1:B:133:LEU:HD12	1:B:283:LYS:HG3	1.87	0.57
1:A:188:GLN:HA	1:A:230:PHE:HB3	1.85	0.57
1:A:250:THR:HG22	1:A:360:PHE:CE1	2.39	0.57
1:B:10:VAL:HA	1:B:164:ALA:O	2.03	0.57
1:B:164:ALA:HA	1:B:186:SER:O	2.05	0.57
1:A:159:TRP:O	1:A:189:HIS:HA	2.04	0.57
1:A:17:LYS:NZ	1:A:356:ALA:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLN:HA	1:A:224:ILE:HD11	1.87	0.57
1:A:242:THR:HG22	1:B:244:ARG:NH2	2.19	0.56
1:B:23:SER:HB3	1:B:41:CYS:SG	2.45	0.56
1:B:161:ARG:HE	1:B:190:SER:HA	1.70	0.56
1:B:27:LEU:HD13	1:B:31:LEU:HD21	1.87	0.56
1:A:159:TRP:CD2	1:A:193:ILE:HG13	2.40	0.56
1:B:171:GLN:HG3	1:B:178:VAL:HG13	1.87	0.56
1:B:367:TRP:O	1:B:368:GLU:HG3	2.06	0.56
1:B:122:MET:SD	1:B:122:MET:N	2.78	0.56
1:A:276:TYR:HE1	1:A:359:HIS:HD2	1.52	0.56
1:B:378:ASP:O	1:B:382:LEU:HD23	2.06	0.56
1:A:84:PHE:HD2	1:A:235:PRO:HD2	1.70	0.56
1:B:11:SER:HA	1:B:357:TYR:CE1	2.41	0.56
1:B:152:ARG:HH22	1:B:162:PRO:HG3	1.71	0.56
1:B:272:ARG:NH2	1:B:354:THR:HG21	2.21	0.56
1:A:118:ASP:HA	1:A:302:ILE:HA	1.87	0.55
1:A:285:ILE:HA	1:A:376:LEU:HD23	1.89	0.55
1:A:37:ALA:HA	1:A:57:THR:O	2.06	0.55
1:A:46:LYS:HA	1:A:235:PRO:HB3	1.89	0.55
1:B:127:THR:HB	1:B:129:GLU:HB2	1.89	0.55
1:B:335:LEU:HA	1:B:340:LEU:HD21	1.88	0.55
1:B:296:ILE:HA	1:B:311:MET:O	2.07	0.55
1:A:177:ILE:HG13	1:A:215:TRP:HZ2	1.71	0.55
1:A:121:LEU:HB2	1:A:297:GLN:NE2	2.18	0.54
1:A:276:TYR:HE1	1:A:359:HIS:CD2	2.24	0.54
1:A:308:THR:HG23	1:B:221:LYS:NZ	2.23	0.54
1:B:18:ILE:HD11	1:B:72:VAL:HG22	1.88	0.54
1:A:320:VAL:HG23	1:A:321:PRO:O	2.07	0.54
1:A:159:TRP:CZ3	1:A:198:LEU:HG	2.42	0.54
1:A:259:GLY:N	1:B:247:ILE:HG21	2.22	0.54
1:B:140:TYR:O	1:B:144:LEU:HB2	2.08	0.54
1:A:259:GLY:HA2	1:B:247:ILE:HB	1.90	0.54
1:A:156:THR:HG22	1:A:157:LEU:HD12	1.90	0.53
1:A:40:ALA:HA	1:A:264:GLY:O	2.08	0.53
1:B:56:ILE:HG13	1:B:95:ILE:HD12	1.91	0.53
1:A:280:TYR:O	1:A:284:ASN:HB2	2.08	0.53
1:A:22:ILE:HD13	1:A:50:VAL:HG11	1.90	0.53
1:B:245:LYS:O	1:B:249:ASP:HB2	2.08	0.53
1:B:272:ARG:HH21	1:B:354:THR:HG21	1.72	0.53
1:A:82:MET:O	1:A:232:ILE:HA	2.09	0.53
1:A:320:VAL:HG21	1:A:324:GLN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:TYR:CE1	1:A:341:ILE:HD12	2.43	0.53
1:B:246:ILE:HB	1:B:257:HIS:HE1	1.74	0.53
1:B:43:THR:HG22	1:B:52:VAL:HA	1.91	0.53
1:A:157:LEU:HB2	1:A:160:LEU:HD11	1.91	0.53
1:B:117:GLY:O	1:B:302:ILE:HG13	2.08	0.53
1:A:202:VAL:HA	1:A:206:ILE:HG12	1.90	0.52
1:B:278:ALA:HA	1:B:281:VAL:CG2	2.37	0.52
1:A:133:LEU:HD21	1:A:287:ALA:HB2	1.92	0.52
1:B:18:ILE:HG21	1:B:235:PRO:HG3	1.91	0.52
1:B:15:PRO:O	1:B:18:ILE:HG22	2.09	0.52
1:B:41:CYS:HA	1:B:54:GLY:HA3	1.91	0.52
1:A:257:HIS:O	1:B:247:ILE:HG13	2.10	0.52
1:A:324:GLN:HG3	1:A:327:LEU:HD12	1.91	0.52
1:B:30:ILE:HG23	1:B:58:THR:HG21	1.92	0.52
1:B:57:THR:HG22	1:B:98:GLN:HB3	1.92	0.52
1:A:172:TYR:CE1	1:A:177:ILE:HG22	2.44	0.51
1:A:298:VAL:HG21	1:A:335:LEU:HD22	1.92	0.51
1:A:247:ILE:HB	1:B:259:GLY:HA2	1.92	0.51
1:A:121:LEU:HG	1:A:258:GLY:HA3	1.93	0.51
1:A:83:GLY:CA	1:A:236:MET:HB2	2.41	0.51
1:A:261:ALA:HB3	1:A:265:LYS:HZ1	1.76	0.51
1:A:300:TYR:CE1	1:A:307:PRO:HB3	2.45	0.51
1:B:44:TYR:HB3	1:B:51:LEU:HD21	1.92	0.51
1:A:3:HIS:HB2	1:A:172:TYR:HB2	1.93	0.50
1:A:242:THR:HG22	1:B:244:ARG:HH21	1.75	0.50
1:B:69:ARG:HH11	1:B:69:ARG:HG2	1.75	0.50
1:A:157:LEU:HD12	1:A:157:LEU:N	2.26	0.50
1:B:170:PHE:CE1	1:B:180:ILE:HD12	2.46	0.50
1:B:189:HIS:O	1:B:231:VAL:HG23	2.11	0.50
1:A:147:ARG:O	1:A:151:VAL:HG22	2.12	0.50
1:B:121:LEU:C	1:B:122:MET:SD	2.89	0.50
1:A:374:GLN:O	1:A:377:ARG:HG3	2.12	0.50
1:B:194:ASP:O	1:B:197:SER:HB3	2.11	0.50
1:B:325:LEU:HA	1:B:328:LEU:HB3	1.93	0.50
1:A:133:LEU:HD13	1:A:283:LYS:HE3	1.94	0.50
1:A:64:ILE:HG22	1:A:68:THR:OG1	2.12	0.50
1:B:202:VAL:HG13	1:B:206:ILE:CG2	2.41	0.50
1:B:8:GLU:HG3	1:B:248:VAL:HG11	1.94	0.50
1:A:245:LYS:HG3	1:A:248:VAL:HG11	1.95	0.49
1:A:276:TYR:HB3	1:A:367:TRP:HB3	1.95	0.49
1:A:324:GLN:O	1:A:327:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HG22	1:A:68:THR:HG1	1.77	0.49
1:B:57:THR:O	1:B:58:THR:HB	2.13	0.49
1:B:161:ARG:HH22	1:B:231:VAL:HG22	1.77	0.49
1:B:144:LEU:HD11	1:B:207:ILE:HA	1.95	0.49
1:B:147:ARG:HB2	1:B:210:ILE:HD11	1.95	0.49
1:A:115:GLY:H	1:A:305:ALA:HB3	1.77	0.49
1:A:116:ALA:N	1:A:305:ALA:HB2	2.28	0.49
1:A:188:GLN:HB2	1:A:230:PHE:HD2	1.77	0.49
1:A:70:ASN:HA	1:A:73:ARG:HD2	1.94	0.49
1:A:224:ILE:HD12	1:A:225:ASN:HB2	1.94	0.48
1:A:70:ASN:O	1:A:73:ARG:HB2	2.13	0.48
1:A:61:TRP:CZ3	1:A:97:LYS:HD3	2.48	0.48
1:B:186:SER:HA	1:B:225:ASN:HB3	1.96	0.48
1:A:34:ASP:HB3	1:A:58:THR:HB	1.94	0.48
1:B:118:ASP:HA	1:B:302:ILE:HB	1.93	0.48
1:B:17:LYS:HA	1:B:17:LYS:HD3	1.77	0.48
1:B:31:LEU:HB3	1:B:349:PRO:HD3	1.95	0.48
1:A:27:LEU:HD13	1:A:39:VAL:CG2	2.43	0.48
1:B:125:TYR:HE2	1:B:135:PRO:HB3	1.79	0.48
1:B:247:ILE:HG23	1:B:252:GLY:O	2.13	0.48
1:B:17:LYS:HD2	1:B:355:ALA:O	2.13	0.48
1:B:169:THR:HB	1:B:182:ALA:HB3	1.95	0.48
1:B:124:GLY:HA3	1:B:278:ALA:O	2.14	0.48
1:B:26:VAL:HG21	1:B:64:ILE:HG22	1.96	0.48
1:A:53:GLY:HA3	1:B:44:TYR:OH	2.14	0.47
1:B:185:LEU:HD13	1:B:207:ILE:HD12	1.94	0.47
1:B:35:PRO:HB2	1:B:347:LEU:HG	1.95	0.47
1:B:37:ALA:HB1	1:B:57:THR:O	2.14	0.47
1:A:15:PRO:HG3	1:A:238:ASP:OD2	2.15	0.47
1:A:66:GLU:O	1:A:70:ASN:HB2	2.15	0.47
1:B:333:PHE:CE1	1:B:372:LYS:HD2	2.49	0.47
1:B:161:ARG:NE	1:B:190:SER:HA	2.29	0.47
1:B:262:PHE:HE1	1:B:275:ALA:HB3	1.80	0.47
1:A:211:LEU:HA	1:A:212:PRO:HD3	1.72	0.47
1:B:138:ILE:HD11	1:B:248:VAL:O	2.15	0.47
1:A:27:LEU:HA	1:A:30:ILE:HG22	1.97	0.47
1:A:77:TYR:HB3	1:A:84:PHE:O	2.13	0.47
1:B:239:CYS:SG	1:B:240:GLY:N	2.87	0.47
1:B:31:LEU:HD12	1:B:35:PRO:HA	1.96	0.47
1:B:23:SER:OG	1:B:43:THR:HG23	2.15	0.47
1:A:7:SER:HB2	1:A:137:PRO:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLU:HA	1:B:166:SER:O	2.15	0.46
1:B:277:ALA:HA	1:B:344:LEU:HD21	1.96	0.46
1:A:245:LYS:HA	1:A:245:LYS:CE	2.45	0.46
1:B:276:TYR:CE1	1:B:359:HIS:HB3	2.37	0.46
1:B:132:VAL:HG13	1:B:134:MET:H	1.80	0.46
1:A:4:LEU:O	1:B:309:SER:HB3	2.15	0.46
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.80	0.46
1:B:262:PHE:CE1	1:B:275:ALA:HB3	2.50	0.46
1:B:33:GLN:OE1	1:B:60:ALA:HA	2.15	0.46
1:B:44:TYR:HB3	1:B:51:LEU:CD2	2.45	0.46
1:B:161:ARG:NH2	1:B:231:VAL:HG22	2.31	0.46
1:B:295:GLU:HG2	1:B:315:PHE:CE1	2.48	0.46
1:A:9:SER:HB2	1:A:141:ALA:CB	2.46	0.45
1:B:182:ALA:HB2	1:B:221:LYS:HD3	1.98	0.45
1:B:5:PHE:CZ	1:B:254:MET:SD	3.09	0.45
1:B:277:ALA:O	1:B:280:TYR:N	2.50	0.45
1:B:27:LEU:O	1:B:31:LEU:HD22	2.16	0.45
1:A:305:ALA:HB1	1:A:336:ARG:HB2	1.97	0.45
1:B:31:LEU:CB	1:B:349:PRO:HD3	2.46	0.45
1:A:152:ARG:HD2	1:A:162:PRO:HG3	1.97	0.45
1:A:174:ASP:C	1:A:176:LYS:H	2.20	0.45
1:A:337:PRO:O	1:A:340:LEU:HD22	2.17	0.45
1:B:152:ARG:NH2	1:B:162:PRO:HG3	2.30	0.45
1:B:77:TYR:OH	1:B:234:GLY:HA2	2.16	0.45
1:B:357:TYR:N	1:B:362:ARG:NH2	2.63	0.45
1:B:22:ILE:HG21	1:B:68:THR:HG23	1.98	0.45
1:A:320:VAL:HG22	1:A:325:LEU:HD12	1.98	0.45
1:B:202:VAL:HA	1:B:206:ILE:HG22	1.99	0.45
1:B:131:ASP:OD1	1:B:132:VAL:HG12	2.17	0.45
1:B:127:THR:O	1:B:133:LEU:HA	2.16	0.45
1:B:328:LEU:HD13	1:B:380:ALA:HB2	1.99	0.45
1:A:24:ASP:OD1	1:A:264:GLY:N	2.50	0.45
1:B:91:VAL:O	1:B:92:LEU:HD23	2.17	0.45
1:A:261:ALA:HB3	1:A:265:LYS:HZ2	1.78	0.45
1:A:333:PHE:CD1	1:A:333:PHE:N	2.85	0.45
1:A:338:TYR:CD1	1:A:341:ILE:HD12	2.52	0.45
1:B:325:LEU:HB2	1:B:328:LEU:HD22	1.99	0.45
1:A:167:GLN:HB3	1:A:184:VAL:CG2	2.47	0.44
1:A:20:ASP:HB3	1:A:355:ALA:HB1	1.99	0.44
1:A:276:TYR:CE1	1:A:359:HIS:CD2	3.05	0.44
1:B:296:ILE:HD11	1:B:298:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ILE:HD12	1:B:257:HIS:ND1	2.33	0.44
1:A:306:GLU:HA	1:A:307:PRO:HD3	1.83	0.44
1:B:300:TYR:CD2	1:B:337:PRO:HG3	2.53	0.44
1:B:46:LYS:HB3	1:B:239:CYS:SG	2.57	0.44
1:A:222:PHE:N	1:A:222:PHE:CD1	2.85	0.44
1:A:236:MET:SD	1:A:236:MET:O	2.76	0.44
1:B:280:TYR:CE2	1:B:343:MET:SD	3.11	0.44
1:B:70:ASN:O	1:B:73:ARG:HB3	2.18	0.44
1:A:74:GLU:OE2	1:A:352:LYS:HD2	2.18	0.44
1:B:163:ASP:O	1:B:187:THR:HA	2.18	0.44
1:B:144:LEU:HD11	1:B:207:ILE:HG13	2.00	0.44
1:B:225:ASN:HA	1:B:226:PRO:HD2	1.82	0.44
1:B:280:TYR:HE2	1:B:343:MET:SD	2.41	0.44
1:A:267:PRO:O	1:A:341:ILE:HD11	2.17	0.44
1:A:79:HIS:H	1:A:82:MET:HE3	1.82	0.44
1:B:246:ILE:HB	1:B:257:HIS:CE1	2.53	0.43
1:B:247:ILE:O	1:B:250:THR:N	2.51	0.43
1:A:210:ILE:HD13	1:A:210:ILE:HA	1.95	0.43
1:A:213:ALA:HA	1:A:216:LEU:HD12	2.00	0.43
1:B:281:VAL:HG21	1:B:296:ILE:HD12	1.99	0.43
1:B:64:ILE:HD11	1:B:93:SER:OG	2.19	0.43
1:B:140:TYR:HD1	1:B:143:ARG:HG3	1.82	0.43
1:B:77:TYR:CZ	1:B:162:PRO:HG2	2.51	0.43
1:B:134:MET:HG3	1:B:135:PRO:CD	2.43	0.43
1:B:140:TYR:CD1	1:B:143:ARG:HG3	2.53	0.43
1:A:127:THR:HG23	1:A:129:GLU:H	1.84	0.43
1:A:69:ARG:HD2	1:A:86:ALA:O	2.19	0.43
1:B:152:ARG:CB	1:B:160:LEU:HD11	2.43	0.43
1:B:188:GLN:HA	1:B:230:PHE:HB3	2.00	0.43
1:A:334:ASP:HB3	1:A:336:ARG:NE	2.34	0.43
1:B:27:LEU:HD13	1:B:31:LEU:CD2	2.47	0.43
1:A:136:ALA:N	1:A:137:PRO:HD2	2.33	0.42
1:A:320:VAL:CG2	1:A:324:GLN:HB3	2.49	0.42
1:B:139:THR:O	1:B:143:ARG:HG2	2.19	0.42
1:B:251:TYR:HE1	1:B:279:ARG:HH21	1.67	0.42
1:B:54:GLY:O	1:B:95:ILE:HA	2.19	0.42
1:A:64:ILE:O	1:A:64:ILE:HG22	2.19	0.42
1:B:288:ALA:HB2	1:B:373:ALA:HB1	2.01	0.42
1:A:268:SER:HB2	1:A:338:TYR:OH	2.20	0.42
1:A:64:ILE:HG21	1:A:64:ILE:HD13	1.80	0.42
1:B:84:PHE:CD2	1:B:235:PRO:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASP:HB2	1:A:267:PRO:CD	2.45	0.42
1:A:26:VAL:CG2	1:A:64:ILE:HG23	2.50	0.42
1:B:134:MET:SD	1:B:279:ARG:NH1	2.93	0.42
1:B:338:TYR:O	1:B:341:ILE:HB	2.19	0.42
1:A:61:TRP:HZ3	1:A:97:LYS:HD3	1.82	0.42
1:B:211:LEU:HA	1:B:212:PRO:HD3	1.71	0.42
1:A:308:THR:HG23	1:B:221:LYS:HZ2	1.83	0.42
1:A:217:THR:HB	1:A:218:SER:H	1.73	0.42
1:A:115:GLY:N	1:A:305:ALA:HB3	2.34	0.42
1:A:365:PHE:HB2	1:A:368:GLU:HB2	2.02	0.42
1:B:40:ALA:HA	1:B:264:GLY:O	2.20	0.42
1:B:294:CYS:SG	1:B:295:GLU:N	2.93	0.42
1:A:133:LEU:HD12	1:A:133:LEU:N	2.35	0.42
1:A:68:THR:HG21	1:A:91:VAL:CG2	2.50	0.42
1:A:183:VAL:HG11	1:A:211:LEU:HD22	2.02	0.41
1:A:18:ILE:HD11	1:A:75:ILE:HD11	2.02	0.41
1:A:250:THR:HG22	1:A:360:PHE:CZ	2.55	0.41
1:B:46:LYS:HB3	1:B:239:CYS:HG	1.85	0.41
1:B:15:PRO:O	1:B:18:ILE:N	2.54	0.41
1:A:123:PHE:CD2	1:A:297:GLN:HB2	2.55	0.41
1:A:217:THR:CB	1:A:219:ALA:H	2.34	0.41
1:A:9:SER:OG	1:A:142:HIS:HA	2.21	0.41
1:A:213:ALA:HA	1:A:216:LEU:HB2	2.03	0.41
1:A:170:PHE:CZ	1:A:180:ILE:HD12	2.55	0.41
1:A:311:MET:HG2	1:B:3:HIS:CG	2.56	0.41
1:A:358:GLY:N	1:A:362:ARG:HH22	2.18	0.41
1:A:87:ASN:OD1	1:A:87:ASN:N	2.54	0.41
1:B:10:VAL:HB	1:B:14:HIS:HB3	2.01	0.41
1:A:350:ILE:HD12	1:A:350:ILE:HA	1.92	0.41
1:B:161:ARG:NH1	1:B:161:ARG:HG3	2.36	0.41
1:B:15:PRO:HG3	1:B:235:PRO:HA	2.03	0.41
1:B:12:GLU:O	1:B:75:ILE:HG21	2.20	0.41
1:B:98:GLN:HB2	1:B:98:GLN:HE21	1.80	0.41
1:A:154:ASN:N	1:A:154:ASN:HD22	2.18	0.41
1:A:377:ARG:HB2	1:A:383:LYS:HA	2.03	0.41
1:A:3:HIS:O	1:A:172:TYR:N	2.53	0.41
1:A:6:THR:HG23	1:A:169:THR:HG22	2.02	0.41
1:A:362:ARG:HD2	1:A:364:HIS:HE1	1.86	0.41
1:B:199:GLN:O	1:B:202:VAL:HB	2.21	0.41
1:A:1:ALA:O	1:A:3:HIS:ND1	2.54	0.40
1:B:193:ILE:HD11	1:B:197:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:MET:SD	1:A:161:ARG:HD2	2.60	0.40
1:A:83:GLY:HA2	1:A:236:MET:HG2	2.02	0.40
1:B:288:ALA:HB3	1:B:290:LEU:HD11	2.02	0.40
1:A:304:VAL:HG12	1:A:306:GLU:O	2.22	0.40
1:B:279:ARG:NH1	1:B:283:LYS:NZ	2.69	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	381/383 (100%)	303 (80%)	69 (18%)	9 (2%)	7	39
1	B	381/383 (100%)	295 (77%)	71 (19%)	15 (4%)	3	25
All	All	762/766 (100%)	598 (78%)	140 (18%)	24 (3%)	5	31

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	B	136	ALA
1	A	228	GLY
1	B	47	THR
1	B	227	THR
1	B	231	VAL
1	B	241	LEU
1	B	350	ILE
1	A	60	ALA
1	A	110	ASP
1	A	115	GLY
1	A	252	GLY
1	B	100	PRO

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Mol	Chain	Res	Type
1	B	110	ASP
1	B	218	SER
1	B	254	MET
1	B	322	SER
1	B	334	ASP
1	B	158	PRO
1	B	267	PRO
1	A	259	GLY
1	B	321	PRO
1	A	137	PRO
1	A	349	PRO

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	311/311 (100%)	236 (76%)	75 (24%)	1	3
1	B	311/311 (100%)	226 (73%)	85 (27%)	0	1
All	All	622/622 (100%)	462 (74%)	160 (26%)	0	2

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	SER
1	A	10	VAL
1	A	12	GLU
1	A	17	LYS
1	A	38	ARG
1	A	41	CYS
1	A	43	THR
1	A	45	VAL
1	A	46	LYS
1	A	61	TRP
1	A	67	ILE

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Mol	Chain	Res	Type
1	A	69	ARG
1	A	78	VAL
1	A	80	SER
1	A	84	PHE
1	A	85	ASP
1	A	87	ASN
1	A	88	SER
1	A	99	SER
1	A	104	GLN
1	A	107	ASP
1	A	108	ARG
1	A	118	ASP
1	A	121	LEU
1	A	127	THR
1	A	131	ASP
1	A	132	VAL
1	A	139	THR
1	A	145	VAL
1	A	152	ARG
1	A	154	ASN
1	A	157	LEU
1	A	160	LEU
1	A	163	ASP
1	A	177	ILE
1	A	194	ASP
1	A	196	LYS
1	A	198	LEU
1	A	206	ILE
1	A	210	ILE
1	A	214	GLU
1	A	218	SER
1	A	224	ILE
1	A	236	MET
1	A	241	LEU
1	A	244	ARG
1	A	245	LYS
1	A	246	ILE
1	A	247	ILE
1	A	248	VAL
1	A	249	ASP
1	A	251	TYR
1	A	262	PHE

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Mol	Chain	Res	Type
1	A	267	PRO
1	A	273	SER
1	A	285	ILE
1	A	296	ILE
1	A	311	MET
1	A	315	PHE
1	A	317	THR
1	A	318	GLU
1	A	330	ARG
1	A	333	PHE
1	A	335	LEU
1	A	336	ARG
1	A	340	LEU
1	A	342	GLN
1	A	344	LEU
1	A	347	LEU
1	A	349	PRO
1	A	360	PHE
1	A	363	GLU
1	A	376	LEU
1	A	377	ARG
1	B	5	PHE
1	B	9	SER
1	B	15	PRO
1	B	18	ILE
1	B	28	ASP
1	B	31	LEU
1	B	38	ARG
1	B	39	VAL
1	B	41	CYS
1	B	55	GLU
1	B	63	ASP
1	B	64	ILE
1	B	70	ASN
1	B	75	ILE
1	B	81	ASP
1	B	84	PHE
1	B	93	SER
1	B	98	GLN
1	B	101	ASP
1	B	106	VAL
1	B	107	ASP

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Mol	Chain	Res	Type
1	B	110	ASP
1	B	118	ASP
1	B	119	GLN
1	B	121	LEU
1	B	127	THR
1	B	130	THR
1	B	131	ASP
1	B	134	MET
1	B	139	THR
1	B	142	HIS
1	B	146	GLN
1	B	148	GLN
1	B	158	PRO
1	B	159	TRP
1	B	161	ARG
1	B	172	TYR
1	B	174	ASP
1	B	177	ILE
1	B	184	VAL
1	B	185	LEU
1	B	188	GLN
1	B	189	HIS
1	B	192	GLU
1	B	194	ASP
1	B	198	LEU
1	B	203	MET
1	B	205	GLU
1	B	207	ILE
1	B	211	LEU
1	B	218	SER
1	B	222	PHE
1	B	225	ASN
1	B	227	THR
1	B	247	ILE
1	B	262	PHE
1	B	263	SER
1	B	268	SER
1	B	279	ARG
1	B	281	VAL
1	B	283	LYS
1	B	284	ASN
1	B	290	LEU

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Mol	Chain	Res	Type
1	B	292	ASP
1	B	296	ILE
1	B	308	THR
1	B	310	ILE
1	B	311	MET
1	B	312	VAL
1	B	314	THR
1	B	315	PHE
1	B	317	THR
1	B	318	GLU
1	B	320	VAL
1	B	325	LEU
1	B	328	LEU
1	B	331	GLU
1	B	332	PHE
1	B	336	ARG
1	B	347	LEU
1	B	352	LYS
1	B	360	PHE
1	B	362	ARG
1	B	364	HIS
1	B	369	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	104	GLN
1	A	142	HIS
1	A	154	ASN
1	A	297	GLN
1	B	98	GLN
1	B	257	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.