



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:31 AM UTC

PDB ID : 1TE0 / pdb_00001te0
Title : Structural analysis of DegS, a stress sensor of the bacterial periplasm
Authors : Ravelli, R.B.G.; Zeth, K.
Deposited on : 2004-05-24
Resolution : 2.20 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

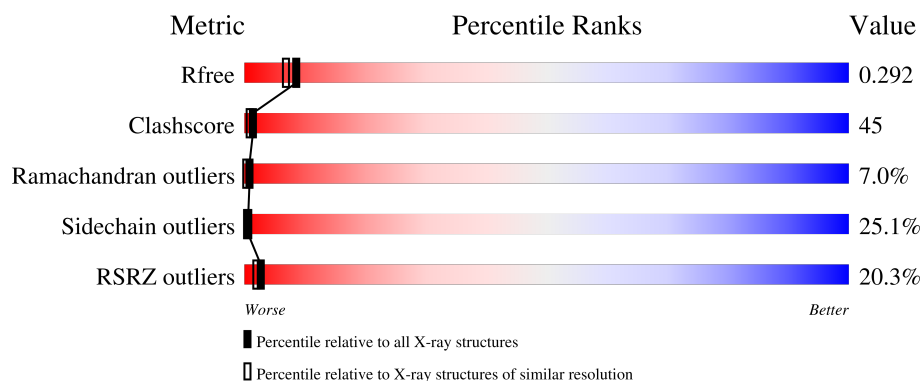
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	318	16% 39% 31% 20% 10%
1	B	318	24% 32% 38% 20% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4829 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 Protease degS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2333	1453	419	456	5			
1	B	318	Total	C	N	O	S	0	0	0
			2333	1453	419	456	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	ILE	LYS	conflict	UNP P31137
A	133	LYS	ASN	conflict	UNP P31137
B	131	ILE	LYS	conflict	UNP P31137
B	133	LYS	ASN	conflict	UNP P31137

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		
2	B	77	Total	O	0	0
			77	77		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	166.28Å 166.28Å 166.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.62 – 2.20 32.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.62-2.20) 99.0 (32.62-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.245 , 0.295 0.243 , 0.292	Depositor DCC
R_{free} test set	1927 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4829	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	2.39	91/2362 (3.9%)	2.11	104/3216 (3.2%)
1	B	2.44	105/2362 (4.4%)	2.14	101/3216 (3.1%)
All	All	2.42	196/4724 (4.1%)	2.12	205/6432 (3.2%)

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	1	8
1	B	1	6
All	All	2	14

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	MET	SD-CE	-21.24	1.26	1.79
1	B	245	MET	SD-CE	-15.36	1.41	1.79
1	A	148	VAL	N-CA	14.61	1.57	1.46
1	A	200	ASN	CA-CB	14.33	1.77	1.54
1	B	104	ILE	CA-CB	11.90	1.68	1.54
1	B	167	THR	CA-CB	11.59	1.68	1.53
1	A	167	THR	CA-CB	10.99	1.67	1.53
1	A	88	ARG	N-CA	10.94	1.60	1.46
1	B	92	ILE	C-O	10.70	1.38	1.24
1	A	322	VAL	CA-CB	10.47	1.66	1.54
1	A	202	GLY	N-CA	10.33	1.63	1.45
1	A	197	ASN	CB-CG	-10.19	1.26	1.52
1	B	305	ILE	CA-CB	10.16	1.67	1.54
1	A	83	VAL	C-O	-10.08	1.13	1.24
1	B	202	GLY	C-O	10.03	1.34	1.23
1	B	200	ASN	CA-CB	9.80	1.70	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	MET	SD-CE	9.65	2.03	1.79
1	B	216	ASN	N-CA	9.63	1.58	1.46
1	B	336	MET	SD-CE	9.11	2.02	1.79
1	A	104	ILE	CA-CB	8.88	1.64	1.54
1	A	214	GLY	C-O	8.87	1.34	1.24
1	B	244	ILE	CA-CB	8.84	1.66	1.54
1	B	228	THR	CA-CB	8.80	1.67	1.53
1	B	242	THR	CB-CG2	-8.69	1.23	1.52
1	A	200	ASN	CB-CG	-8.28	1.31	1.52
1	A	215	ILE	CA-CB	8.28	1.63	1.54
1	A	243	LYS	C-O	8.14	1.33	1.24
1	B	202	GLY	N-CA	8.13	1.59	1.45
1	A	244	ILE	CA-CB	8.08	1.64	1.54
1	B	304	ILE	CA-CB	8.05	1.63	1.54
1	A	326	ARG	CA-C	8.03	1.62	1.53
1	B	90	TYR	CA-C	7.84	1.63	1.52
1	B	249	ILE	CA-C	7.81	1.62	1.52
1	B	271	ALA	CA-CB	7.77	1.64	1.53
1	A	256	ARG	CD-NE	7.73	1.57	1.46
1	B	254	VAL	CA-CB	7.72	1.63	1.53
1	A	197	ASN	CA-CB	7.67	1.67	1.53
1	A	168	ILE	CG1-CD1	-7.65	1.22	1.51
1	A	151	ILE	CA-C	7.58	1.61	1.52
1	B	151	ILE	C-O	7.56	1.32	1.24
1	A	312	ALA	CA-CB	7.51	1.62	1.52
1	A	150	HIS	CA-C	7.50	1.61	1.52
1	B	241	ALA	CA-CB	7.50	1.65	1.53
1	B	322	VAL	CA-CB	7.45	1.64	1.54
1	A	200	ASN	CG-OD1	7.43	1.37	1.23
1	A	221	ASP	CA-C	7.42	1.61	1.52
1	B	131	ILE	CA-CB	7.40	1.64	1.54
1	B	148	VAL	CA-C	7.37	1.58	1.53
1	A	106	VAL	CA-CB	7.37	1.63	1.54
1	B	340	LYS	CA-C	7.36	1.61	1.52
1	B	129	VAL	CA-CB	7.33	1.64	1.54
1	B	172	ILE	CA-CB	7.25	1.65	1.54
1	A	325	ILE	CA-CB	7.23	1.63	1.54
1	B	52	ARG	NE-CZ	7.21	1.41	1.33
1	A	202	GLY	CA-C	7.20	1.63	1.51
1	B	200	ASN	CG-OD1	7.17	1.37	1.23
1	A	173	ILE	CA-CB	7.16	1.62	1.53
1	B	168	ILE	CA-CB	-7.14	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	THR	CB-CG2	-7.02	1.29	1.52
1	B	182	ASN	N-CA	6.99	1.56	1.46
1	A	233	GLY	CA-C	6.97	1.60	1.52
1	B	190	LEU	C-O	6.97	1.32	1.23
1	B	55	ALA	N-CA	6.96	1.55	1.46
1	B	183	PRO	CA-C	6.93	1.59	1.52
1	A	168	ILE	C-O	-6.90	1.16	1.24
1	A	120	GLY	CA-C	6.83	1.58	1.51
1	A	206	VAL	CA-CB	6.82	1.66	1.54
1	B	172	ILE	C-O	6.81	1.31	1.23
1	B	217	THR	CA-CB	-6.80	1.42	1.53
1	B	86	ASP	N-CA	6.79	1.53	1.46
1	B	200	ASN	CB-CG	-6.70	1.35	1.52
1	B	83	VAL	CB-CG2	6.66	1.74	1.52
1	B	227	GLU	N-CA	6.66	1.55	1.46
1	A	52	ARG	NE-CZ	6.63	1.40	1.33
1	B	173	ILE	C-O	6.58	1.30	1.24
1	B	86	ASP	C-O	6.52	1.31	1.23
1	B	193	ASP	N-CA	-6.52	1.38	1.46
1	A	147	ARG	C-O	-6.50	1.16	1.23
1	A	192	THR	C-O	-6.49	1.15	1.23
1	B	50	ALA	CA-CB	6.39	1.63	1.53
1	B	219	SER	CB-OG	6.39	1.54	1.42
1	B	148	VAL	CA-CB	6.34	1.61	1.54
1	A	216	ASN	C-O	6.31	1.31	1.23
1	A	219	SER	CA-CB	6.30	1.64	1.53
1	A	321	GLN	C-O	-6.29	1.16	1.24
1	A	178	ARG	CG-CD	6.26	1.71	1.52
1	B	147	ARG	CD-NE	-6.25	1.37	1.46
1	B	247	LYS	CG-CD	-6.24	1.33	1.52
1	B	90	TYR	CE2-CZ	6.24	1.53	1.38
1	B	70	SER	CA-C	6.20	1.61	1.52
1	B	276	ILE	CA-CB	6.17	1.62	1.54
1	B	227	GLU	CA-C	6.15	1.61	1.52
1	B	78	THR	CA-C	6.14	1.59	1.52
1	A	240	LEU	CA-C	6.13	1.60	1.52
1	A	157	ALA	CA-C	6.12	1.60	1.52
1	A	103	GLN	CA-C	6.12	1.59	1.52
1	A	98	ILE	CA-C	6.11	1.60	1.52
1	B	332	PRO	C-O	6.08	1.30	1.23
1	A	115	GLU	CA-C	6.08	1.60	1.52
1	B	115	GLU	C-O	6.07	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	THR	C-O	6.07	1.31	1.23
1	B	168	ILE	CG1-CD1	-6.07	1.28	1.51
1	B	197	ASN	CB-CG	-6.03	1.36	1.52
1	A	148	VAL	CA-CB	6.03	1.60	1.53
1	A	55	ALA	CA-CB	6.01	1.62	1.53
1	A	87	GLN	C-N	-6.01	1.25	1.33
1	A	158	ILE	C-O	-5.99	1.17	1.24
1	A	37	PHE	N-CA	5.98	1.57	1.46
1	A	122	ASP	C-O	5.93	1.30	1.23
1	A	222	LYS	CA-C	5.89	1.60	1.52
1	A	222	LYS	N-CA	5.86	1.53	1.46
1	A	239	GLN	N-CA	5.85	1.53	1.46
1	B	81	SER	N-CA	5.84	1.52	1.45
1	A	227	GLU	CA-C	5.82	1.60	1.52
1	B	163	ASN	C-O	5.81	1.31	1.24
1	B	124	LEU	CA-C	-5.81	1.45	1.52
1	B	234	PHE	CA-C	-5.77	1.45	1.52
1	B	178	ARG	CA-C	-5.74	1.46	1.52
1	B	222	LYS	N-CA	5.72	1.53	1.46
1	B	253	ARG	C-O	5.68	1.29	1.24
1	A	225	ASP	N-CA	5.68	1.55	1.46
1	B	201	SER	CB-OG	-5.67	1.30	1.42
1	B	262	GLY	CA-C	5.64	1.56	1.52
1	A	337	ARG	CA-C	5.62	1.59	1.52
1	B	113	VAL	CA-CB	5.60	1.63	1.55
1	A	122	ASP	CA-C	5.59	1.58	1.52
1	A	241	ALA	CA-C	5.58	1.60	1.52
1	B	141	ILE	CA-CB	5.57	1.61	1.53
1	A	154	VAL	CA-CB	5.56	1.60	1.54
1	B	130	LEU	N-CA	-5.55	1.39	1.45
1	A	50	ALA	N-CA	5.52	1.53	1.46
1	A	293	ALA	CA-CB	-5.51	1.44	1.53
1	B	235	ALA	C-O	5.49	1.30	1.23
1	B	168	ILE	CB-CG2	-5.49	1.34	1.52
1	B	194	ALA	CA-CB	5.48	1.61	1.53
1	A	253	ARG	CA-C	5.46	1.59	1.52
1	A	93	THR	C-O	-5.45	1.18	1.24
1	A	330	VAL	CA-CB	5.43	1.60	1.54
1	B	147	ARG	NE-CZ	5.43	1.39	1.33
1	B	67	ASN	CA-C	5.43	1.59	1.52
1	A	57	ALA	N-CA	-5.42	1.39	1.46
1	A	105	ILE	CA-CB	5.42	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	ILE	CA-CB	5.41	1.61	1.54
1	B	257	GLY	CA-C	5.39	1.57	1.52
1	A	133	LYS	C-O	-5.39	1.17	1.24
1	B	107	ALA	N-CA	5.37	1.52	1.46
1	B	58	VAL	CA-CB	5.37	1.60	1.54
1	A	350	GLU	C-O	-5.35	1.17	1.23
1	B	87	GLN	C-N	-5.34	1.26	1.33
1	B	101	ALA	C-O	-5.34	1.17	1.23
1	B	255	ILE	CA-CB	5.32	1.60	1.54
1	A	59	VAL	CB-CG2	-5.32	1.35	1.52
1	A	219	SER	CB-OG	5.32	1.52	1.42
1	A	319	MET	CG-SD	5.31	1.94	1.80
1	B	240	LEU	CG-CD2	5.31	1.70	1.52
1	B	330	VAL	CA-C	-5.31	1.45	1.52
1	B	156	LEU	CA-C	-5.30	1.46	1.52
1	A	276	ILE	CA-CB	5.30	1.61	1.54
1	A	348	ILE	CA-C	5.30	1.58	1.52
1	A	212	LEU	CA-C	5.29	1.60	1.52
1	B	94	ASN	CA-CB	5.29	1.61	1.53
1	B	320	ASP	CG-OD1	5.28	1.35	1.25
1	B	48	ASN	CG-OD1	5.27	1.33	1.23
1	B	103	GLN	C-O	5.27	1.29	1.23
1	A	305	ILE	CA-C	5.26	1.59	1.53
1	B	154	VAL	CB-CG1	5.26	1.70	1.52
1	B	161	PRO	CA-C	5.25	1.59	1.52
1	A	183	PRO	C-O	-5.25	1.17	1.24
1	B	85	MET	SD-CE	-5.24	1.66	1.79
1	A	235	ALA	N-CA	-5.23	1.39	1.45
1	A	144	ASN	CB-CG	5.21	1.65	1.52
1	B	293	ALA	CA-C	5.21	1.59	1.52
1	A	215	ILE	CB-CG2	5.20	1.69	1.52
1	B	267	ALA	N-CA	5.20	1.53	1.46
1	A	152	GLY	C-O	5.19	1.31	1.24
1	B	84	ILE	N-CA	5.14	1.52	1.46
1	A	189	PHE	CA-C	5.14	1.58	1.52
1	B	123	SER	C-O	-5.13	1.18	1.24
1	B	141	ILE	CA-C	-5.13	1.48	1.52
1	A	156	LEU	C-O	5.13	1.30	1.24
1	B	352	PRO	CA-C	5.11	1.59	1.52
1	A	182	ASN	CB-CG	5.10	1.64	1.52
1	B	171	GLY	C-O	5.09	1.28	1.24
1	B	83	VAL	CA-C	5.09	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	ASN	CA-C	5.08	1.59	1.52
1	B	47	TYR	CA-C	5.06	1.60	1.52
1	A	307	VAL	CA-CB	5.05	1.60	1.54
1	B	326	ARG	CD-NE	5.05	1.53	1.46
1	B	339	ASP	CA-C	5.05	1.59	1.52
1	A	220	PHE	CA-C	5.03	1.59	1.52
1	B	157	ALA	CA-C	5.03	1.59	1.52
1	B	244	ILE	CG1-CD1	-5.03	1.32	1.51
1	A	161	PRO	CA-C	5.03	1.59	1.52
1	B	225	ASP	N-CA	5.02	1.54	1.46
1	B	222	LYS	CA-C	5.01	1.58	1.52
1	A	127	LEU	CG-CD2	5.01	1.69	1.52

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASP	N-CA-C	15.93	133.26	111.92
1	B	225	ASP	N-CA-C	14.53	131.39	111.92
1	B	201	SER	CA-C-N	-12.80	89.47	121.60
1	B	201	SER	C-N-CA	-12.80	89.47	121.60
1	A	200	ASN	CA-CB-CG	-12.78	99.82	112.60
1	B	87	GLN	N-CA-C	-12.77	94.70	110.41
1	B	168	ILE	N-CA-C	12.41	126.11	108.36
1	B	201	SER	CA-CB-OG	-12.39	86.32	111.10
1	A	201	SER	CA-C-N	-12.18	91.03	121.60
1	A	201	SER	C-N-CA	-12.18	91.03	121.60
1	A	168	ILE	N-CA-C	11.89	124.82	108.17
1	B	200	ASN	CA-CB-CG	-11.85	100.75	112.60
1	B	227	GLU	N-CA-C	11.33	125.27	109.18
1	B	222	LYS	N-CA-C	11.14	126.89	108.73
1	A	222	LYS	N-CA-C	10.91	126.51	108.73
1	B	166	GLN	N-CA-C	10.52	125.69	108.96
1	A	87	GLN	O-C-N	-9.87	110.50	122.65
1	A	201	SER	O-C-N	-9.57	111.97	122.12
1	B	143	ILE	N-CA-C	9.54	122.68	108.46
1	A	161	PRO	N-CA-C	9.46	131.96	112.47
1	A	166	GLN	N-CA-C	9.36	123.83	108.96
1	A	224	ASN	CA-C-N	9.24	135.84	122.35
1	A	224	ASN	C-N-CA	9.24	135.84	122.35
1	B	161	PRO	N-CA-C	9.10	131.22	112.47
1	A	227	GLU	N-CA-C	8.95	123.02	109.41
1	B	201	SER	O-C-N	-8.74	111.52	122.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	LEU	CA-C-N	-8.72	109.89	122.19
1	B	74	LEU	C-N-CA	-8.72	109.89	122.19
1	A	244	ILE	CA-CB-CG2	8.68	125.25	110.50
1	B	295	ASN	N-CA-C	-8.64	97.53	110.24
1	B	135	THR	N-CA-C	8.35	128.58	110.80
1	A	247	LYS	CD-CE-NZ	-8.28	85.41	111.90
1	B	132	ILE	CA-CB-CG2	8.22	124.47	110.50
1	A	305	ILE	CB-CA-C	8.19	118.27	111.06
1	A	87	GLN	CA-C-N	-8.18	105.91	121.54
1	A	87	GLN	C-N-CA	-8.18	105.91	121.54
1	A	104	ILE	CB-CA-C	8.11	122.08	110.98
1	B	244	ILE	CB-CG1-CD1	-8.10	96.79	113.80
1	A	242	THR	N-CA-CB	-8.05	98.29	110.12
1	A	132	ILE	CA-CB-CG2	7.99	124.08	110.50
1	A	244	ILE	CB-CG1-CD1	-7.92	97.18	113.80
1	A	85	MET	N-CA-C	7.89	122.18	112.23
1	A	286	GLU	N-CA-C	-7.83	96.17	109.24
1	B	74	LEU	N-CA-C	7.74	127.28	110.80
1	A	305	ILE	N-CA-C	-7.72	105.24	112.96
1	B	104	ILE	CA-CB-CG2	7.68	123.56	110.50
1	B	202	GLY	N-CA-C	7.67	124.82	115.31
1	B	244	ILE	CA-CB-CG2	7.65	123.50	110.50
1	B	328	GLY	N-CA-C	-7.64	104.99	114.92
1	B	340	LYS	N-CA-C	7.59	121.28	108.90
1	A	88	ARG	CB-CA-C	-7.55	95.39	110.42
1	B	353	ALA	N-CA-C	7.53	120.03	110.24
1	B	224	ASN	CA-C-N	7.32	133.04	122.35
1	B	224	ASN	C-N-CA	7.32	133.04	122.35
1	B	71	HIS	N-CA-C	7.24	126.22	110.80
1	B	93	THR	CB-CA-C	-7.21	96.07	110.42
1	A	98	ILE	N-CA-C	7.17	123.85	113.16
1	B	187	GLN	N-CA-C	-7.16	101.73	112.54
1	A	200	ASN	CB-CG-ND2	7.15	127.13	116.40
1	A	323	ALA	N-CA-C	7.06	119.88	111.33
1	A	93	THR	CB-CA-C	-7.04	96.93	114.11
1	B	192	THR	CA-CB-CG2	7.02	122.44	110.50
1	B	190	LEU	CA-CB-CG	7.00	140.80	116.30
1	A	192	THR	CA-CB-OG1	6.89	119.93	109.60
1	A	300	VAL	N-CA-C	6.89	123.66	109.34
1	A	200	ASN	CB-CG-OD1	-6.88	107.04	120.80
1	B	91	ILE	CA-C-N	-6.87	113.08	122.91
1	B	91	ILE	C-N-CA	-6.87	113.08	122.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	PHE	N-CA-C	6.84	125.38	110.80
1	A	179	ILE	N-CA-CB	-6.82	103.29	112.22
1	A	74	LEU	N-CA-C	6.81	121.61	111.81
1	A	146	ARG	NE-CZ-NH1	-6.77	114.73	121.50
1	A	178	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	B	192	THR	CB-CA-C	-6.69	96.06	110.45
1	A	350	GLU	N-CA-CB	6.67	120.13	110.06
1	B	104	ILE	CB-CA-C	6.66	120.75	110.83
1	A	296	ALA	N-CA-C	6.65	124.97	110.80
1	A	285	ASN	CB-CA-C	-6.58	100.00	110.86
1	A	87	GLN	N-CA-C	-6.58	102.05	110.53
1	B	332	PRO	CA-C-N	-6.56	114.37	123.10
1	B	332	PRO	C-N-CA	-6.56	114.37	123.10
1	B	200	ASN	CB-CG-ND2	6.47	126.10	116.40
1	A	71	HIS	N-CA-C	6.45	124.54	110.80
1	B	83	VAL	N-CA-C	6.42	117.10	107.80
1	A	113	VAL	CB-CA-C	6.37	120.11	110.62
1	A	303	LEU	N-CA-C	6.37	124.36	110.80
1	B	167	THR	OG1-CB-CG2	-6.35	96.60	109.30
1	A	178	ARG	CG-CD-NE	-6.33	98.08	112.00
1	B	192	THR	CA-CB-OG1	6.31	119.06	109.60
1	A	337	ARG	N-CA-C	6.26	121.00	112.68
1	B	220	PHE	N-CA-C	6.24	124.10	110.80
1	B	178	ARG	NE-CZ-NH1	-6.24	115.27	121.50
1	B	38	ASP	O-C-N	-6.20	115.25	122.87
1	A	309	ASN	N-CA-C	6.19	120.07	111.90
1	B	196	ILE	CA-C-N	6.17	132.21	122.21
1	B	196	ILE	C-N-CA	6.17	132.21	122.21
1	A	200	ASN	N-CA-C	6.16	121.12	112.93
1	A	62	TYR	N-CA-C	6.15	119.50	109.59
1	A	201	SER	CA-CB-OG	-6.11	98.88	111.10
1	A	141	ILE	N-CA-C	6.10	115.60	108.96
1	B	197	ASN	CB-CA-C	-6.04	96.78	110.07
1	B	296	ALA	N-CA-C	6.02	123.62	110.80
1	B	166	GLN	CB-CA-C	-6.01	100.18	110.22
1	B	200	ASN	CB-CG-OD1	-6.00	108.80	120.80
1	A	237	PRO	CA-C-N	-6.00	111.19	120.31
1	A	237	PRO	C-N-CA	-6.00	111.19	120.31
1	B	166	GLN	CA-C-N	-5.95	115.11	122.84
1	B	166	GLN	C-N-CA	-5.95	115.11	122.84
1	B	353	ALA	CA-C-N	5.95	132.40	121.70
1	B	353	ALA	C-N-CA	5.95	132.40	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	LEU	N-CA-C	-5.93	100.04	109.23
1	A	143	ILE	N-CA-C	5.91	116.80	108.17
1	A	79	LEU	CA-CB-CG	5.89	136.93	116.30
1	A	302	ASP	N-CA-C	5.89	119.53	112.93
1	A	59	VAL	N-CA-CB	-5.88	99.73	111.91
1	B	217	THR	N-CA-C	5.85	117.94	108.34
1	A	43	THR	CA-CB-OG1	-5.84	100.84	109.60
1	A	48	ASN	N-CA-C	-5.84	105.41	112.54
1	B	350	GLU	N-CA-C	5.84	119.43	110.20
1	B	224	ASN	N-CA-C	5.84	123.24	110.80
1	B	242	THR	CA-CB-CG2	5.82	120.40	110.50
1	B	160	ASN	CA-C-N	5.82	127.11	119.84
1	B	160	ASN	C-N-CA	5.82	127.11	119.84
1	A	326	ARG	CA-C-O	5.82	125.22	119.75
1	B	87	GLN	O-C-N	-5.81	115.57	122.65
1	A	131	ILE	N-CA-C	5.80	118.32	108.86
1	A	193	ASP	CA-C-N	-5.80	112.83	120.95
1	A	193	ASP	C-N-CA	-5.80	112.83	120.95
1	B	169	THR	N-CA-C	5.78	118.97	109.72
1	A	295	ASN	N-CA-C	-5.78	101.75	110.24
1	A	197	ASN	CB-CA-C	-5.77	97.81	110.67
1	B	38	ASP	CB-CA-C	-5.77	101.62	111.31
1	A	124	LEU	N-CA-C	-5.71	105.19	111.82
1	A	346	VAL	N-CA-C	5.67	116.65	108.48
1	B	251	ASP	CB-CG-OD2	5.66	131.42	118.40
1	B	213	MET	N-CA-C	-5.66	106.73	113.97
1	B	134	ALA	N-CA-C	5.62	118.70	109.72
1	B	337	ARG	N-CA-C	5.60	120.38	112.93
1	A	104	ILE	CA-CB-CG2	5.57	119.96	110.50
1	A	332	PRO	CA-C-O	-5.54	115.17	121.98
1	A	93	THR	CA-CB-OG1	5.53	117.89	109.60
1	A	338	ASP	N-CA-C	-5.52	99.40	109.56
1	A	201	SER	N-CA-CB	5.50	118.21	110.12
1	A	179	ILE	N-CA-C	5.50	117.48	111.77
1	A	346	VAL	CA-C-N	-5.48	115.48	122.77
1	A	346	VAL	C-N-CA	-5.48	115.48	122.77
1	B	193	ASP	N-CA-C	-5.46	105.83	112.88
1	B	59	VAL	CA-CB-CG1	5.44	119.64	110.40
1	B	164	LEU	N-CA-C	5.44	116.95	107.49
1	A	147	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	B	183	PRO	N-CA-C	5.42	120.32	114.68
1	B	241	ALA	N-CA-C	-5.40	105.47	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	THR	CA-CB-CG2	5.40	119.68	110.50
1	B	132	ILE	CB-CG1-CD1	-5.39	102.48	113.80
1	A	190	LEU	CA-CB-CG	5.37	135.10	116.30
1	A	216	ASN	N-CA-CB	5.35	117.87	109.69
1	B	75	GLU	N-CA-C	5.34	118.33	109.46
1	B	261	ILE	N-CA-C	-5.33	101.24	108.06
1	B	38	ASP	CA-C-N	-5.33	113.05	122.26
1	B	38	ASP	C-N-CA	-5.33	113.05	122.26
1	A	218	LEU	CA-C-O	5.26	126.21	120.95
1	A	182	ASN	CB-CA-C	-5.24	101.69	109.60
1	A	160	ASN	CA-C-N	5.23	126.38	119.84
1	A	160	ASN	C-N-CA	5.23	126.38	119.84
1	B	351	TYR	O-C-N	5.21	125.66	121.38
1	B	351	TYR	CB-CA-C	-5.20	101.55	109.50
1	B	330	VAL	CB-CA-C	-5.19	104.24	110.99
1	B	260	GLY	CA-C-N	5.18	129.88	121.95
1	B	260	GLY	C-N-CA	5.18	129.88	121.95
1	A	195	SER	N-CA-CB	5.18	117.51	109.48
1	A	324	GLU	CA-C-N	-5.16	115.71	122.37
1	A	324	GLU	C-N-CA	-5.16	115.71	122.37
1	B	167	THR	CB-CA-C	5.16	119.03	110.78
1	A	353	ALA	N-CA-C	5.16	117.57	110.35
1	A	74	LEU	CB-CA-C	-5.15	104.85	111.50
1	B	242	THR	N-CA-CB	-5.15	102.54	110.01
1	A	167	THR	OG1-CB-CG2	-5.14	99.01	109.30
1	A	325	ILE	N-CA-CB	5.13	116.32	110.72
1	B	253	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	194	ALA	CA-C-O	-5.12	114.93	120.81
1	A	134	ALA	CA-C-N	5.11	130.75	122.07
1	A	134	ALA	C-N-CA	5.11	130.75	122.07
1	A	66	LEU	N-CA-C	5.10	116.58	108.67
1	B	73	GLN	CA-C-N	5.09	131.26	121.54
1	B	73	GLN	C-N-CA	5.09	131.26	121.54
1	B	158	ILE	N-CA-C	5.08	115.29	108.17
1	B	200	ASN	N-CA-C	5.08	119.68	112.93
1	A	60	ASN	CA-C-N	-5.07	116.36	123.10
1	A	60	ASN	C-N-CA	-5.07	116.36	123.10
1	B	322	VAL	N-CA-C	-5.07	105.60	110.72
1	B	303	LEU	CA-CB-CG	5.07	134.04	116.30
1	A	224	ASN	N-CA-C	5.07	121.59	110.80
1	B	217	THR	CA-C-N	5.07	128.04	120.95
1	B	217	THR	C-N-CA	5.07	128.04	120.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	VAL	CA-C-N	-5.06	116.04	122.37
1	B	333	VAL	C-N-CA	-5.06	116.04	122.37
1	A	55	ALA	N-CA-C	5.05	120.97	109.81
1	A	196	ILE	CA-C-N	5.04	130.43	122.36
1	A	196	ILE	C-N-CA	5.04	130.43	122.36
1	B	334	VAL	N-CA-CB	5.04	116.74	111.00
1	B	341	GLN	CA-C-N	-5.04	115.09	122.19
1	B	341	GLN	C-N-CA	-5.04	115.09	122.19
1	A	190	LEU	N-CA-CB	-5.03	102.92	110.17
1	A	327	PRO	CA-C-O	-5.01	115.63	121.34
1	A	242	THR	CB-CA-C	5.00	119.09	110.79

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	192	THR	CB
1	B	192	THR	CB

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	GLY	Peptide
1	A	159	GLY	Peptide
1	A	163	ASN	Peptide
1	A	197	ASN	Mainchain
1	A	218	LEU	Peptide
1	A	220	PHE	Peptide
1	A	70	SER	Peptide
1	A	73	GLN	Peptide
1	B	136	GLY	Peptide
1	B	163	ASN	Peptide
1	B	202	GLY	Peptide
1	B	218	LEU	Peptide
1	B	220	PHE	Peptide
1	B	73	GLN	Peptide

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	2333	0	2356	182	2
1	B	2333	0	2356	237	1
2	A	86	0	0	43	1
2	B	77	0	0	41	2
All	All	4829	0	4712	419	3

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 45.

All (419) 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:83:VAL:CG2	1:B:83:VAL:CB	1.74	1.63
1:A:200:ASN:CB	1:A:200:ASN:CA	1.77	1.59
1:B:336:MET:SD	1:B:336:MET:CE	2.02	1.47
1:A:213:MET:SD	1:A:213:MET:CE	2.03	1.44
1:A:231:GLY:HA3	2:A:421:HOH:O	1.16	1.31
1:A:69:ASN:HB3	2:A:385:HOH:O	1.33	1.27
1:B:160:ASN:HB2	1:B:161:PRO:CD	1.74	1.18
1:A:87:GLN:O	1:A:88:ARG:CB	1.85	1.17
1:A:87:GLN:O	1:A:88:ARG:HB2	1.43	1.14
1:A:160:ASN:N	1:A:160:ASN:HD22	1.40	1.13
1:A:146:ARG:HG2	1:A:146:ARG:HH11	1.12	1.12
1:B:220:PHE:HE2	2:B:404:HOH:O	1.29	1.12
1:B:146:ARG:HG2	1:B:146:ARG:NH1	1.49	1.11
1:B:337:ARG:HG3	1:B:337:ARG:HH11	1.10	1.11
1:B:161:PRO:HB2	1:B:199:GLY:HA2	1.36	1.08
1:B:178:ARG:NH2	1:B:317:GLU:OE1	1.88	1.07
1:B:88:ARG:N	2:B:381:HOH:O	1.69	1.07
1:A:79:LEU:HD21	2:A:415:HOH:O	1.55	1.06
1:A:200:ASN:OD1	1:A:200:ASN:HA	1.53	1.05
1:A:276:ILE:HA	2:A:384:HOH:O	1.55	1.05
1:A:166:GLN:HG3	2:A:406:HOH:O	1.56	1.04
1:A:274:GLY:H	1:A:275:GLY:HA2	1.17	1.04
1:A:266:ILE:HD11	1:A:303:LEU:HD21	1.40	1.03
1:B:146:ARG:HH11	1:B:146:ARG:CG	1.71	1.03
1:A:284:VAL:O	1:A:300:VAL:O	1.74	1.03
1:A:220:PHE:N	2:A:435:HOH:O	1.90	1.02
1:B:274:GLY:H	1:B:275:GLY:HA2	1.19	1.02
1:A:192:THR:HG22	1:A:194:ALA:H	1.23	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:CD2	2:A:415:HOH:O	2.10	1.00
1:A:94:ASN:HD21	1:A:201:SER:HB2	1.26	0.99
1:A:200:ASN:CA	1:A:200:ASN:OD1	2.08	0.99
1:B:160:ASN:HA	1:B:166:GLN:HA	1.44	0.99
1:B:38:ASP:CG	1:B:38:ASP:O	2.07	0.98
1:A:160:ASN:N	1:A:160:ASN:ND2	2.08	0.97
1:A:160:ASN:HB2	1:A:161:PRO:CD	1.93	0.97
1:B:160:ASN:HB2	1:B:161:PRO:HD3	1.45	0.96
1:A:200:ASN:CA	1:A:200:ASN:CG	2.38	0.96
1:B:146:ARG:HG2	1:B:146:ARG:HH11	0.83	0.96
1:A:337:ARG:HG3	1:A:337:ARG:HH11	1.27	0.96
1:B:160:ASN:N	1:B:160:ASN:HD22	1.64	0.94
1:B:284:VAL:HB	1:B:300:VAL:O	1.68	0.94
1:B:94:ASN:HD21	1:B:201:SER:HB2	1.31	0.93
1:A:160:ASN:HD22	1:A:160:ASN:H	1.16	0.93
1:B:69:ASN:HD22	1:B:69:ASN:H	1.08	0.93
1:A:69:ASN:H	1:A:69:ASN:HD22	1.02	0.93
1:B:135:THR:HA	2:B:372:HOH:O	1.68	0.92
1:B:247:LYS:HE2	2:B:361:HOH:O	1.69	0.90
1:A:133:LYS:HE3	2:A:375:HOH:O	1.70	0.90
1:B:319:MET:HB3	2:B:393:HOH:O	1.72	0.90
1:B:198:HIS:CB	1:B:225:ASP:CB	2.48	0.90
1:A:178:ARG:HD3	2:A:365:HOH:O	1.72	0.90
1:A:146:ARG:HG2	1:A:146:ARG:NH1	1.79	0.90
1:B:41:ASP:HB2	2:B:382:HOH:O	1.73	0.89
1:B:94:ASN:ND2	1:B:201:SER:HB2	1.87	0.88
1:A:38:ASP:OD1	1:A:38:ASP:O	1.91	0.88
1:A:310:LYS:CE	2:A:419:HOH:O	2.20	0.88
1:B:52:ARG:NH2	2:B:392:HOH:O	1.77	0.88
1:B:271:ALA:HB1	2:B:405:HOH:O	1.74	0.88
1:B:280:GLN:HG3	1:B:281:GLY:H	1.39	0.88
1:A:168:ILE:HG21	2:A:410:HOH:O	1.73	0.87
1:B:87:GLN:CA	2:B:381:HOH:O	2.22	0.87
1:B:198:HIS:HB2	1:B:225:ASP:CB	2.03	0.87
1:B:337:ARG:HG3	1:B:337:ARG:NH1	1.82	0.87
1:A:161:PRO:HG3	2:A:415:HOH:O	1.75	0.87
1:B:67:ASN:ND2	1:B:69:ASN:ND2	2.23	0.87
1:B:165:GLY:HA2	2:B:426:HOH:O	1.74	0.87
1:A:79:LEU:CD2	1:A:161:PRO:HG3	2.04	0.87
1:A:222:LYS:O	1:A:223:SER:HB2	1.74	0.86
1:B:295:ASN:N	1:B:295:ASN:HD22	1.74	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLN:O	1:B:88:ARG:HB2	1.72	0.85
1:B:67:ASN:ND2	1:B:69:ASN:HD22	1.75	0.85
1:B:79:LEU:HD22	1:B:161:PRO:HG3	1.59	0.85
1:B:81:SER:O	1:B:202:GLY:HA3	1.75	0.85
1:B:298:ILE:HG12	1:B:344:LEU:HD12	1.58	0.84
1:B:160:ASN:HB2	1:B:161:PRO:HD2	1.59	0.83
1:B:271:ALA:O	1:B:273:GLY:N	2.11	0.83
1:B:67:ASN:HD22	1:B:69:ASN:HD22	1.26	0.83
1:A:160:ASN:HB2	1:A:161:PRO:HD3	1.60	0.83
1:A:81:SER:O	1:A:202:GLY:HA3	1.79	0.83
1:B:119:VAL:CG2	1:B:131:ILE:HG22	2.08	0.83
1:A:182:ASN:HD22	1:A:182:ASN:N	1.77	0.82
1:B:104:ILE:C	1:B:104:ILE:HD12	2.04	0.82
1:B:192:THR:HG22	1:B:194:ALA:H	1.44	0.82
1:B:69:ASN:H	1:B:69:ASN:ND2	1.77	0.82
1:A:201:SER:HB3	1:A:218:LEU:H	1.44	0.82
1:A:87:GLN:O	1:A:88:ARG:CG	2.27	0.82
1:A:162:TYR:HA	2:A:407:HOH:O	1.80	0.82
1:B:271:ALA:HB2	2:B:394:HOH:O	1.77	0.82
1:A:182:ASN:HB2	2:A:425:HOH:O	1.80	0.82
1:B:38:ASP:O	1:B:38:ASP:OD1	1.97	0.82
1:A:198:HIS:HB2	1:A:225:ASP:CB	2.09	0.81
1:A:274:GLY:N	1:A:275:GLY:HA2	1.94	0.81
1:B:71:HIS:HB2	2:B:396:HOH:O	1.80	0.81
1:A:182:ASN:HD22	1:A:182:ASN:H	1.25	0.81
1:B:160:ASN:N	1:B:160:ASN:ND2	2.26	0.81
1:B:295:ASN:HD22	1:B:295:ASN:H	1.26	0.81
1:A:198:HIS:CB	1:A:225:ASP:CB	2.58	0.80
1:A:161:PRO:CG	2:A:415:HOH:O	2.28	0.80
1:A:319:MET:CE	2:A:425:HOH:O	2.29	0.80
1:A:302:ASP:CG	1:A:337:ARG:HH12	1.88	0.80
1:A:319:MET:HE3	2:A:425:HOH:O	1.80	0.80
1:A:71:HIS:O	1:A:72:ASN:HB2	1.78	0.80
1:A:172:ILE:O	1:A:192:THR:HG23	1.82	0.79
1:A:310:LYS:HE2	2:A:419:HOH:O	1.81	0.79
1:B:326:ARG:O	1:B:329:SER:OG	1.99	0.79
1:B:198:HIS:HB3	1:B:225:ASP:CB	2.11	0.78
1:B:274:GLY:N	1:B:275:GLY:HA2	1.95	0.78
1:B:160:ASN:CB	1:B:161:PRO:CD	2.56	0.78
1:B:83:VAL:CG2	1:B:83:VAL:CA	2.62	0.78
1:B:146:ARG:NH1	1:B:146:ARG:CG	2.34	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:VAL:HG13	1:B:301:ASN:H	1.48	0.78
1:B:131:ILE:HD11	2:B:360:HOH:O	1.84	0.77
1:B:266:ILE:HD11	1:B:281:GLY:HA3	1.66	0.77
1:B:87:GLN:O	1:B:88:ARG:CB	2.23	0.77
1:A:119:VAL:CG2	1:A:131:ILE:HG22	2.15	0.77
1:B:266:ILE:HD11	1:B:303:LEU:HD23	1.66	0.77
1:A:94:ASN:ND2	1:A:201:SER:HB2	1.98	0.77
1:B:83:VAL:CG2	1:B:83:VAL:CG1	2.62	0.77
1:B:295:ASN:H	1:B:295:ASN:ND2	1.78	0.76
1:A:302:ASP:CB	1:A:337:ARG:NH1	2.49	0.76
1:B:242:THR:HG21	2:B:377:HOH:O	1.84	0.76
1:A:220:PHE:HA	2:A:429:HOH:O	1.86	0.76
1:A:295:ASN:O	1:A:296:ALA:HB3	1.84	0.76
1:B:219:SER:HB2	2:B:401:HOH:O	1.84	0.76
1:B:71:HIS:O	1:B:72:ASN:HB2	1.85	0.76
1:B:72:ASN:O	1:B:73:GLN:HB2	1.83	0.76
1:B:160:ASN:O	1:B:165:GLY:O	2.04	0.76
1:B:186:ARG:HG3	1:B:186:ARG:HH11	1.50	0.75
1:B:299:GLN:HA	2:B:413:HOH:O	1.86	0.75
1:B:198:HIS:HB3	1:B:225:ASP:O	1.87	0.74
1:A:69:ASN:HD22	1:A:69:ASN:N	1.78	0.74
1:A:168:ILE:CG2	2:A:410:HOH:O	2.34	0.73
1:A:198:HIS:HB3	1:A:225:ASP:O	1.88	0.73
1:A:79:LEU:HD22	1:A:161:PRO:HG3	1.71	0.72
1:A:88:ARG:HD3	2:A:434:HOH:O	1.88	0.72
1:B:266:ILE:HD11	1:B:303:LEU:CD2	2.19	0.72
1:B:198:HIS:NE2	2:B:430:HOH:O	2.23	0.72
1:A:67:ASN:ND2	1:A:69:ASN:O	2.22	0.71
1:A:161:PRO:HD3	2:A:415:HOH:O	1.91	0.71
1:A:168:ILE:HB	2:A:410:HOH:O	1.91	0.71
1:A:266:ILE:CD1	1:A:303:LEU:HD21	2.18	0.71
1:A:69:ASN:H	1:A:69:ASN:ND2	1.84	0.70
1:B:333:VAL:HG12	2:B:399:HOH:O	1.92	0.69
1:B:300:VAL:HG13	1:B:301:ASN:N	2.08	0.69
1:B:197:ASN:H	1:B:200:ASN:HB2	1.57	0.69
1:A:71:HIS:C	1:A:72:ASN:HD22	2.01	0.69
1:A:168:ILE:CB	2:A:410:HOH:O	2.41	0.68
1:B:135:THR:O	1:B:136:GLY:C	2.36	0.68
1:B:135:THR:CG2	2:B:372:HOH:O	2.41	0.68
1:A:266:ILE:HD11	1:A:303:LEU:CD2	2.21	0.68
1:A:295:ASN:O	1:A:296:ALA:CB	2.40	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLN:CG	1:B:281:GLY:H	2.05	0.68
1:A:160:ASN:HA	1:A:166:GLN:HA	1.76	0.68
1:B:303:LEU:HD22	1:B:305:ILE:HD13	1.76	0.68
1:A:182:ASN:HB2	2:A:417:HOH:O	1.94	0.68
1:B:86:ASP:OD1	1:B:87:GLN:O	2.11	0.68
1:B:72:ASN:O	1:B:73:GLN:CB	2.41	0.68
1:B:71:HIS:O	1:B:72:ASN:CB	2.42	0.67
1:B:104:ILE:C	1:B:104:ILE:CD1	2.67	0.67
1:B:280:GLN:HG3	1:B:281:GLY:N	2.10	0.67
1:B:220:PHE:CE2	2:B:404:HOH:O	2.16	0.67
1:A:302:ASP:CB	1:A:337:ARG:HH12	2.08	0.66
1:B:60:ASN:OD1	1:B:160:ASN:CG	2.37	0.66
1:B:135:THR:HG22	2:B:372:HOH:O	1.94	0.66
1:A:104:ILE:HD12	1:A:104:ILE:C	2.21	0.66
1:B:119:VAL:HG23	1:B:131:ILE:HG22	1.76	0.66
1:A:200:ASN:CB	1:A:200:ASN:C	2.66	0.66
1:B:303:LEU:CD2	1:B:305:ILE:HD13	2.26	0.66
1:A:161:PRO:CD	2:A:415:HOH:O	2.41	0.65
1:B:165:GLY:HA3	2:B:425:HOH:O	1.95	0.65
1:A:135:THR:O	1:A:136:GLY:C	2.36	0.65
1:B:335:VAL:HG23	2:B:416:HOH:O	1.95	0.65
1:A:302:ASP:OD2	1:A:337:ARG:NH1	2.26	0.65
1:A:38:ASP:HA	2:A:370:HOH:O	1.96	0.65
1:A:198:HIS:HB3	1:A:225:ASP:CB	2.26	0.65
1:A:146:ARG:NH1	1:A:146:ARG:CG	2.46	0.65
1:B:287:VAL:O	1:B:288:SER:C	2.40	0.65
1:A:71:HIS:O	1:A:72:ASN:CB	2.45	0.65
1:A:229:PRO:O	1:A:230:GLU:CB	2.44	0.65
1:B:294:ALA:O	1:B:297:GLY:HA2	1.96	0.64
1:A:74:LEU:HB2	2:A:393:HOH:O	1.96	0.64
1:B:160:ASN:CB	1:B:161:PRO:HD2	2.22	0.64
1:B:71:HIS:C	1:B:72:ASN:HD22	2.05	0.64
1:B:313:ILE:HG22	1:B:314:SER:HB3	1.80	0.64
1:A:302:ASP:HB3	1:A:337:ARG:NH1	2.13	0.64
1:B:79:LEU:CD2	1:B:161:PRO:HG3	2.28	0.64
1:B:219:SER:HB3	1:B:234:PHE:HD1	1.61	0.63
1:B:326:ARG:HH11	1:B:326:ARG:CG	2.10	0.63
1:A:242:THR:HG21	2:A:432:HOH:O	1.98	0.63
1:B:160:ASN:CA	1:B:166:GLN:HA	2.24	0.63
1:B:289:PRO:O	1:B:290:ASP:C	2.41	0.63
1:B:186:ARG:HH11	1:B:186:ARG:CG	2.12	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASN:O	1:B:300:VAL:HG23	1.98	0.62
1:A:269:LEU:HD23	1:A:269:LEU:H	1.63	0.62
1:A:165:GLY:HA2	2:A:372:HOH:O	1.99	0.62
1:A:292:PRO:O	1:A:295:ASN:O	2.16	0.62
1:B:182:ASN:N	1:B:182:ASN:HD22	1.98	0.62
1:A:119:VAL:HG23	1:A:131:ILE:HG22	1.81	0.62
1:B:298:ILE:CG1	1:B:344:LEU:HD12	2.28	0.62
1:B:186:ARG:HG3	1:B:186:ARG:NH1	2.07	0.62
1:B:119:VAL:CG2	1:B:131:ILE:CG2	2.78	0.61
1:A:280:GLN:HG3	1:A:281:GLY:H	1.63	0.61
1:A:179:ILE:HG13	1:A:240:LEU:HB2	1.82	0.61
1:B:266:ILE:CD1	1:B:303:LEU:CD2	2.78	0.61
1:A:239:GLN:NE2	2:A:432:HOH:O	2.34	0.61
1:B:41:ASP:CB	2:B:382:HOH:O	2.40	0.61
1:A:181:LEU:HD11	1:A:247:LYS:HZ1	1.65	0.60
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.66	0.60
1:A:178:ARG:NH2	1:A:317:GLU:OE1	2.30	0.60
1:B:96:HIS:NE2	2:B:411:HOH:O	2.32	0.60
1:A:61:VAL:HG13	1:A:104:ILE:HD11	1.83	0.60
1:B:313:ILE:O	1:B:314:SER:HB2	2.01	0.60
1:B:302:ASP:HB3	1:B:337:ARG:NH1	2.17	0.60
1:A:160:ASN:HB2	1:A:161:PRO:HD2	1.81	0.59
1:B:294:ALA:N	2:B:383:HOH:O	2.32	0.59
1:A:302:ASP:CG	1:A:337:ARG:NH1	2.61	0.59
1:A:114:PHE:HB2	1:A:132:ILE:HG12	1.84	0.59
1:A:337:ARG:HG3	1:A:337:ARG:NH1	2.03	0.59
1:B:104:ILE:CD1	1:B:105:ILE:N	2.66	0.59
1:B:160:ASN:C	1:B:165:GLY:O	2.45	0.58
1:A:79:LEU:HD23	1:A:161:PRO:HG3	1.86	0.58
1:B:295:ASN:O	1:B:296:ALA:HB3	2.04	0.58
1:B:94:ASN:HD21	1:B:201:SER:CB	2.10	0.58
1:B:298:ILE:HG12	1:B:344:LEU:CD1	2.31	0.58
1:A:104:ILE:HD12	1:A:105:ILE:N	2.19	0.58
1:A:147:ARG:HD2	1:A:211:GLU:OE1	2.04	0.58
1:A:201:SER:O	1:A:202:GLY:C	2.30	0.57
1:B:313:ILE:O	1:B:313:ILE:HG23	2.04	0.57
1:A:192:THR:HG22	1:A:194:ALA:N	2.08	0.57
1:B:266:ILE:HG13	1:B:281:GLY:O	2.05	0.57
1:B:266:ILE:CD1	1:B:303:LEU:HD23	2.32	0.57
1:B:293:ALA:O	1:B:297:GLY:O	2.23	0.57
1:A:166:GLN:HB2	2:A:368:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:N	1:A:182:ASN:ND2	2.41	0.56
1:A:197:ASN:H	1:A:200:ASN:HB2	1.69	0.56
1:B:168:ILE:HG12	1:B:169:THR:N	2.19	0.56
1:A:127:LEU:HD12	1:A:244:ILE:HG12	1.88	0.56
1:A:146:ARG:HH11	1:A:146:ARG:CG	1.86	0.55
1:A:309:ASN:OD1	2:A:403:HOH:O	2.18	0.55
1:B:266:ILE:HD11	1:B:281:GLY:CA	2.33	0.55
1:B:292:PRO:O	1:B:295:ASN:O	2.23	0.55
1:A:73:GLN:HA	1:A:73:GLN:HE21	1.72	0.55
1:B:87:GLN:HA	2:B:381:HOH:O	2.00	0.55
1:A:73:GLN:HA	1:A:73:GLN:NE2	2.21	0.55
1:B:295:ASN:O	1:B:296:ALA:CB	2.54	0.55
1:A:162:TYR:CA	2:A:407:HOH:O	2.46	0.55
1:B:179:ILE:HG23	1:B:179:ILE:O	2.06	0.55
1:A:295:ASN:N	1:A:295:ASN:HD22	2.05	0.55
1:B:104:ILE:HD12	1:B:105:ILE:N	2.21	0.55
1:B:296:ALA:N	1:B:297:GLY:HA2	2.21	0.55
1:B:156:LEU:HD13	1:B:168:ILE:HD11	1.89	0.55
1:A:114:PHE:CB	1:A:132:ILE:HG12	2.37	0.54
1:B:159:GLY:C	1:B:160:ASN:ND2	2.65	0.54
1:B:48:ASN:HD21	1:B:52:ARG:HE	1.55	0.54
1:A:160:ASN:O	1:A:167:THR:N	2.36	0.54
1:A:274:GLY:H	1:A:275:GLY:CA	2.05	0.54
1:A:119:VAL:CG2	1:A:131:ILE:CG2	2.86	0.54
1:B:284:VAL:CB	1:B:300:VAL:O	2.51	0.54
1:A:161:PRO:HB2	1:A:199:GLY:HA2	1.90	0.53
1:B:238:PHE:O	1:B:242:THR:HB	2.08	0.53
1:B:182:ASN:O	1:B:182:ASN:ND2	2.42	0.53
1:A:182:ASN:CG	1:A:320:ASP:OD1	2.52	0.53
1:B:324:GLU:CG	2:B:385:HOH:O	2.56	0.53
1:B:86:ASP:OD1	1:B:88:ARG:HB2	2.09	0.53
1:B:178:ARG:HB2	1:B:188:ASN:HA	1.89	0.53
1:A:284:VAL:HB	1:A:300:VAL:O	2.08	0.53
1:A:67:ASN:HB2	1:A:69:ASN:ND2	2.24	0.52
1:A:160:ASN:CB	1:A:161:PRO:CD	2.72	0.52
1:A:181:LEU:CD1	1:A:247:LYS:HZ1	2.23	0.52
1:A:86:ASP:OD1	1:A:88:ARG:HB2	2.10	0.52
1:A:285:ASN:O	1:A:300:VAL:HG23	2.10	0.52
1:B:197:ASN:O	1:B:200:ASN:N	2.41	0.52
1:B:117:LEU:HD23	1:B:131:ILE:HG23	1.92	0.52
1:B:284:VAL:O	1:B:300:VAL:O	2.28	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ARG:HH11	1:B:337:ARG:CG	1.97	0.52
1:B:59:VAL:HG22	1:B:108:LEU:HD22	1.92	0.52
1:B:94:ASN:HD21	1:B:201:SER:C	2.18	0.52
1:B:69:ASN:O	1:B:70:SER:C	2.53	0.51
1:A:259:ILE:HB	1:A:322:VAL:HG11	1.93	0.51
1:A:310:LYS:NZ	2:A:419:HOH:O	2.41	0.51
1:B:319:MET:CA	2:B:393:HOH:O	2.58	0.51
1:B:67:ASN:ND2	1:B:69:ASN:O	2.43	0.51
1:B:280:GLN:CG	1:B:281:GLY:N	2.73	0.51
1:B:247:LYS:CE	2:B:361:HOH:O	2.40	0.51
1:A:168:ILE:HG12	1:A:169:THR:N	2.24	0.50
1:A:293:ALA:O	1:A:297:GLY:O	2.28	0.50
1:A:159:GLY:C	1:A:160:ASN:ND2	2.70	0.50
1:A:141:ILE:HG12	1:A:212:LEU:HD13	1.93	0.50
1:A:38:ASP:OD1	1:A:38:ASP:C	2.55	0.49
1:A:219:SER:C	2:A:435:HOH:O	2.42	0.49
1:B:67:ASN:HD21	1:B:69:ASN:ND2	2.06	0.49
1:B:87:GLN:HB3	2:B:381:HOH:O	2.11	0.49
1:B:86:ASP:C	1:B:87:GLN:O	2.49	0.49
1:A:197:ASN:HB2	1:A:200:ASN:HB2	1.95	0.49
1:A:181:LEU:N	1:A:182:ASN:HD22	2.11	0.49
1:A:64:ARG:NH1	2:A:393:HOH:O	2.42	0.48
1:A:197:ASN:HB3	1:A:199:GLY:H	1.77	0.48
1:B:293:ALA:C	1:B:295:ASN:O	2.56	0.48
1:B:313:ILE:O	1:B:313:ILE:CG2	2.60	0.48
1:B:326:ARG:HH11	1:B:326:ARG:HG2	1.77	0.48
1:B:104:ILE:HD13	1:B:105:ILE:N	2.28	0.48
1:B:69:ASN:ND2	1:B:69:ASN:N	2.47	0.48
1:B:179:ILE:O	1:B:179:ILE:CG2	2.61	0.48
1:B:266:ILE:HG13	1:B:266:ILE:H	1.21	0.48
1:B:139:PRO:HA	2:B:424:HOH:O	2.13	0.48
1:B:67:ASN:HB3	1:B:72:ASN:HA	1.95	0.48
1:B:192:THR:CG2	1:B:194:ALA:H	2.18	0.48
1:A:302:ASP:OD1	1:A:302:ASP:C	2.56	0.48
1:B:229:PRO:O	1:B:230:GLU:CB	2.61	0.48
1:A:60:ASN:OD1	1:A:160:ASN:CG	2.57	0.47
1:A:182:ASN:CG	1:A:182:ASN:O	2.55	0.47
1:A:85:MET:HG3	1:A:245:MET:HE1	1.96	0.47
1:A:319:MET:HE2	2:A:425:HOH:O	2.02	0.47
1:B:220:PHE:CD1	1:B:220:PHE:N	2.82	0.47
1:B:220:PHE:N	1:B:220:PHE:HD1	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PRO:O	1:A:290:ASP:C	2.56	0.47
1:B:300:VAL:CG1	1:B:301:ASN:H	2.22	0.47
1:B:266:ILE:CD1	1:B:303:LEU:HD21	2.43	0.47
1:B:346:VAL:HG23	1:B:347:THR:N	2.29	0.47
1:B:266:ILE:HG12	1:B:283:VAL:HG22	1.95	0.47
1:B:337:ARG:NH1	1:B:337:ARG:CG	2.62	0.47
1:A:98:ILE:HD12	1:A:98:ILE:C	2.40	0.47
1:A:133:LYS:CE	2:A:375:HOH:O	2.44	0.47
1:A:182:ASN:ND2	1:A:320:ASP:OD1	2.47	0.47
1:B:147:ARG:CD	1:B:211:GLU:OE1	2.64	0.46
1:B:201:SER:O	1:B:202:GLY:C	2.33	0.46
1:A:294:ALA:O	1:A:297:GLY:HA2	2.16	0.46
1:B:71:HIS:C	1:B:72:ASN:ND2	2.74	0.46
1:B:73:GLN:HA	1:B:73:GLN:HE21	1.79	0.46
1:B:95:LYS:HE2	1:B:121:SER:OG	2.15	0.46
1:B:303:LEU:HD13	1:B:336:MET:HB2	1.97	0.46
1:B:63:ASN:OD1	1:B:77:ARG:HD2	2.16	0.46
1:A:247:LYS:HZ3	1:A:247:LYS:HG2	1.51	0.46
1:B:135:THR:CA	2:B:372:HOH:O	2.44	0.46
1:A:52:ARG:HD3	2:A:396:HOH:O	2.17	0.45
1:A:160:ASN:CB	1:A:161:PRO:HD2	2.43	0.45
1:B:69:ASN:O	1:B:70:SER:O	2.34	0.45
1:B:185:GLY:HA3	1:B:188:ASN:HD22	1.81	0.45
1:A:68:THR:HB	2:A:426:HOH:O	2.16	0.45
1:B:135:THR:O	1:B:136:GLY:O	2.34	0.45
1:B:302:ASP:CG	1:B:337:ARG:HH12	2.24	0.45
1:B:59:VAL:CG2	1:B:108:LEU:HD22	2.47	0.45
1:B:298:ILE:CG1	1:B:344:LEU:CD1	2.92	0.45
1:B:324:GLU:HG3	2:B:385:HOH:O	2.16	0.45
1:A:81:SER:O	1:A:93:THR:CG2	2.65	0.45
1:B:326:ARG:HD3	1:B:327:PRO:O	2.17	0.45
1:B:219:SER:O	1:B:220:PHE:HB2	2.17	0.44
1:B:160:ASN:O	1:B:167:THR:N	2.51	0.44
1:A:313:ILE:HD13	1:A:313:ILE:HG21	1.56	0.44
1:B:326:ARG:HH11	1:B:326:ARG:HG3	1.81	0.44
1:A:61:VAL:HG13	1:A:104:ILE:CD1	2.48	0.44
1:A:166:GLN:CG	2:A:406:HOH:O	2.37	0.44
1:B:172:ILE:O	1:B:192:THR:HG23	2.17	0.44
1:B:303:LEU:HD21	1:B:305:ILE:CD1	2.47	0.44
1:A:266:ILE:HG13	1:A:281:GLY:O	2.18	0.44
1:A:326:ARG:HA	1:A:327:PRO:HD3	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASP:CB	1:B:337:ARG:NH1	2.80	0.44
1:B:326:ARG:CG	1:B:326:ARG:NH1	2.77	0.44
1:A:266:ILE:HD11	1:A:281:GLY:HA3	2.00	0.44
1:B:303:LEU:HD21	1:B:305:ILE:HD13	2.00	0.44
1:A:326:ARG:HG2	1:A:327:PRO:HD2	2.00	0.44
1:B:253:ARG:HH11	1:B:253:ARG:HD3	1.57	0.44
1:A:228:THR:O	1:A:229:PRO:O	2.36	0.43
1:A:243:LYS:NZ	1:A:324:GLU:OE2	2.48	0.43
1:A:287:VAL:O	1:A:288:SER:C	2.59	0.43
1:B:69:ASN:HD22	1:B:69:ASN:N	1.88	0.43
1:A:119:VAL:HG21	1:A:131:ILE:HG22	2.00	0.43
1:B:67:ASN:HD22	1:B:69:ASN:H	1.65	0.43
1:B:219:SER:HB3	1:B:234:PHE:CD1	2.48	0.43
1:B:269:LEU:H	1:B:269:LEU:HD23	1.81	0.43
1:B:266:ILE:CD1	1:B:281:GLY:HA3	2.43	0.43
1:B:290:ASP:HA	1:B:295:ASN:HD21	1.82	0.43
1:B:147:ARG:HD3	1:B:211:GLU:OE1	2.18	0.43
1:B:229:PRO:HG2	2:B:401:HOH:O	2.19	0.43
1:B:91:ILE:HD12	1:B:132:ILE:HD13	2.00	0.42
1:A:178:ARG:HH22	1:A:317:GLU:CD	2.23	0.42
1:B:216:ASN:C	1:B:217:THR:HG23	2.44	0.42
1:B:294:ALA:O	1:B:295:ASN:C	2.60	0.42
1:A:147:ARG:CD	1:A:211:GLU:OE1	2.67	0.42
1:A:230:GLU:CB	2:A:422:HOH:O	2.67	0.42
1:B:160:ASN:O	1:B:166:GLN:HA	2.18	0.42
1:B:305:ILE:HD12	1:B:305:ILE:HA	1.88	0.42
1:B:319:MET:HA	2:B:393:HOH:O	2.20	0.42
1:B:266:ILE:CD1	1:B:281:GLY:CA	2.97	0.42
1:B:325:ILE:HG21	1:B:348:ILE:HG13	2.01	0.42
1:B:73:GLN:HA	1:B:73:GLN:NE2	2.34	0.42
1:B:313:ILE:HG22	1:B:314:SER:CB	2.46	0.42
1:B:178:ARG:HH11	1:B:178:ARG:HD3	1.65	0.42
1:B:265:GLU:HA	1:B:281:GLY:O	2.20	0.42
1:B:216:ASN:C	1:B:217:THR:CG2	2.92	0.42
1:B:168:ILE:HD12	1:B:168:ILE:HG21	1.72	0.41
1:A:274:GLY:N	1:A:275:GLY:CA	2.72	0.41
1:B:326:ARG:HG2	1:B:326:ARG:NH1	2.35	0.41
1:B:271:ALA:C	1:B:273:GLY:H	2.27	0.41
1:A:295:ASN:HD22	1:A:295:ASN:H	1.66	0.41
1:B:114:PHE:CB	1:B:132:ILE:HG12	2.50	0.41
1:A:104:ILE:C	1:A:104:ILE:CD1	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:VAL:CG1	1:B:301:ASN:N	2.78	0.41
1:A:259:ILE:O	1:A:292:PRO:HD2	2.20	0.41
1:B:48:ASN:ND2	1:B:52:ARG:HE	2.16	0.41
1:A:87:GLN:NE2	1:A:138:LEU:O	2.54	0.41
1:A:182:ASN:H	1:A:182:ASN:ND2	1.99	0.41
1:A:337:ARG:NH1	1:A:337:ARG:CG	2.77	0.41
1:B:143:ILE:HG21	1:B:143:ILE:HD13	1.78	0.41
1:B:266:ILE:HD12	1:B:280:GLN:C	2.46	0.41
1:B:313:ILE:HD13	1:B:313:ILE:HG21	1.73	0.41
1:A:94:ASN:HD21	1:A:201:SER:CB	2.13	0.41
1:A:228:THR:N	1:A:229:PRO:HD2	2.36	0.41
1:B:87:GLN:O	1:B:88:ARG:CG	2.68	0.41
1:B:214:GLY:HA2	1:B:236:ILE:O	2.20	0.41
1:A:322:VAL:HA	1:A:325:ILE:HD12	2.02	0.40
1:B:271:ALA:CB	2:B:394:HOH:O	2.52	0.40
1:A:180:GLY:C	1:A:182:ASN:ND2	2.80	0.40
1:B:87:GLN:CB	2:B:381:HOH:O	2.59	0.40
1:B:247:LYS:NZ	2:B:361:HOH:O	2.53	0.40
1:B:326:ARG:O	1:B:327:PRO:C	2.64	0.40
1:B:185:GLY:HA3	1:B:188:ASN:ND2	2.35	0.40
1:B:315:ALA:HB3	2:B:420:HOH:O	2.21	0.40
1:B:333:VAL:CG1	2:B:399:HOH:O	2.60	0.40

All (3) 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)
2:A:431:HOH:O	2:B:355:HOH:O[20_555]	1.51	0.69
1:A:88:ARG:NH2	2:B:397:HOH:O[20_555]	2.00	0.20
1:A:146:ARG:NH1	1:B:246:ASP:OD2[20_555]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	316/318 (99%)	272 (86%)	23 (7%)	21 (7%)	1	0
1	B	316/318 (99%)	265 (84%)	28 (9%)	23 (7%)	1	0
All	All	632/636 (99%)	537 (85%)	51 (8%)	44 (7%)	1	0

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	160	ASN
1	A	161	PRO
1	A	220	PHE
1	A	223	SER
1	A	224	ASN
1	A	229	PRO
1	A	230	GLU
1	A	266	ILE
1	A	272	GLN
1	B	72	ASN
1	B	88	ARG
1	B	135	THR
1	B	160	ASN
1	B	161	PRO
1	B	220	PHE
1	B	223	SER
1	B	224	ASN
1	B	229	PRO
1	B	266	ILE
1	B	270	HIS
1	B	272	GLN
1	A	73	GLN
1	A	162	TYR
1	A	163	ASN
1	A	270	HIS
1	A	271	ALA
1	A	296	ALA
1	B	70	SER
1	B	73	GLN
1	B	136	GLY
1	B	162	TYR
1	B	163	ASN
1	B	230	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	280	GLN
1	B	296	ALA
1	B	314	SER
1	A	280	GLN
1	A	298	ILE
1	B	274	GLY
1	A	40	THR
1	B	298	ILE
1	A	136	GLY
1	A	274	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	249/257 (97%)	191 (77%)	58 (23%)	1	0
1	B	249/257 (97%)	182 (73%)	67 (27%)	0	0
All	All	498/514 (97%)	373 (75%)	125 (25%)	0	0

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	59	VAL
1	A	69	ASN
1	A	73	GLN
1	A	75	GLU
1	A	93	THR
1	A	104	ILE
1	A	113	VAL
1	A	131	ILE
1	A	132	ILE
1	A	133	LYS
1	A	135	THR
1	A	143	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	146	ARG
1	A	147	ARG
1	A	160	ASN
1	A	163	ASN
1	A	164	LEU
1	A	167	THR
1	A	168	ILE
1	A	176	THR
1	A	179	ILE
1	A	182	ASN
1	A	184	THR
1	A	186	ARG
1	A	187	GLN
1	A	190	LEU
1	A	195	SER
1	A	201	SER
1	A	220	PHE
1	A	223	SER
1	A	228	THR
1	A	239	GLN
1	A	242	THR
1	A	244	ILE
1	A	247	LYS
1	A	259	ILE
1	A	264	ARG
1	A	266	ILE
1	A	269	LEU
1	A	272	GLN
1	A	278	GLN
1	A	279	LEU
1	A	286	GLU
1	A	288	SER
1	A	290	ASP
1	A	295	ASN
1	A	303	LEU
1	A	305	ILE
1	A	310	LYS
1	A	313	ILE
1	A	314	SER
1	A	316	LEU
1	A	326	ARG
1	A	337	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	LYS
1	A	346	VAL
1	A	350	GLU
1	B	39	SER
1	B	40	THR
1	B	42	GLU
1	B	59	VAL
1	B	67	ASN
1	B	69	ASN
1	B	70	SER
1	B	72	ASN
1	B	73	GLN
1	B	75	GLU
1	B	93	THR
1	B	104	ILE
1	B	108	LEU
1	B	113	VAL
1	B	131	ILE
1	B	132	ILE
1	B	133	LYS
1	B	135	THR
1	B	143	ILE
1	B	146	ARG
1	B	160	ASN
1	B	163	ASN
1	B	164	LEU
1	B	167	THR
1	B	168	ILE
1	B	176	THR
1	B	178	ARG
1	B	179	ILE
1	B	182	ASN
1	B	184	THR
1	B	186	ARG
1	B	190	LEU
1	B	192	THR
1	B	201	SER
1	B	220	PHE
1	B	228	THR
1	B	239	GLN
1	B	242	THR
1	B	244	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	247	LYS
1	B	259	ILE
1	B	264	ARG
1	B	265	GLU
1	B	266	ILE
1	B	269	LEU
1	B	272	GLN
1	B	278	GLN
1	B	279	LEU
1	B	283	VAL
1	B	286	GLU
1	B	290	ASP
1	B	295	ASN
1	B	301	ASN
1	B	303	LEU
1	B	304	ILE
1	B	305	ILE
1	B	310	LYS
1	B	313	ILE
1	B	317	GLU
1	B	319	MET
1	B	326	ARG
1	B	329	SER
1	B	336	MET
1	B	337	ARG
1	B	340	LYS
1	B	346	VAL
1	B	351	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	69	ASN
1	A	72	ASN
1	A	73	GLN
1	A	94	ASN
1	A	160	ASN
1	A	170	GLN
1	A	182	ASN
1	A	188	ASN
1	A	239	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	272	GLN
1	A	295	ASN
1	A	321	GLN
1	B	48	ASN
1	B	67	ASN
1	B	69	ASN
1	B	72	ASN
1	B	73	GLN
1	B	94	ASN
1	B	96	HIS
1	B	160	ASN
1	B	166	GLN
1	B	170	GLN
1	B	182	ASN
1	B	188	ASN
1	B	198	HIS
1	B	272	GLN
1	B	295	ASN
1	B	309	ASN
1	B	321	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 oligosaccharides 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/318 (100%)	1.03	52 (16%) 4 3	33, 54, 81, 85	0
1	B	318/318 (100%)	1.18	77 (24%) 2 1	34, 54, 81, 85	0
All	All	636/636 (100%)	1.11	129 (20%) 3 2	33, 54, 81, 85	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	ASN	8.1
1	B	276	ILE	7.6
1	A	162	TYR	7.2
1	A	271	ALA	6.4
1	A	268	PRO	5.3
1	A	225	ASP	5.2
1	B	267	ALA	5.2
1	B	228	THR	5.1
1	B	271	ALA	5.0
1	B	184	THR	4.9
1	B	162	TYR	4.9
1	B	163	ASN	4.9
1	B	183	PRO	4.8
1	B	229	PRO	4.7
1	A	163	ASN	4.7
1	A	161	PRO	4.7
1	A	186	ARG	4.6
1	B	274	GLY	4.6
1	A	229	PRO	4.6
1	B	164	LEU	4.5
1	A	69	ASN	4.5
1	B	219	SER	4.4
1	A	220	PHE	4.3
1	A	269	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	71	HIS	4.2
1	B	289	PRO	4.2
1	B	268	PRO	4.1
1	A	267	ALA	4.1
1	B	298	ILE	4.1
1	B	37	PHE	4.0
1	A	272	GLN	4.0
1	B	224	ASN	4.0
1	A	266	ILE	4.0
1	B	161	PRO	3.9
1	A	276	ILE	3.9
1	B	269	LEU	3.8
1	A	66	LEU	3.8
1	A	270	HIS	3.7
1	B	354	THR	3.7
1	B	277	ASP	3.7
1	B	38	ASP	3.6
1	B	66	LEU	3.6
1	B	220	PHE	3.5
1	B	273	GLY	3.5
1	A	223	SER	3.5
1	B	165	GLY	3.5
1	B	296	ALA	3.4
1	A	297	GLY	3.4
1	A	222	LYS	3.3
1	A	353	ALA	3.3
1	A	68	THR	3.3
1	B	351	TYR	3.3
1	A	300	VAL	3.3
1	A	279	LEU	3.3
1	B	303	LEU	3.2
1	A	228	THR	3.2
1	B	258	TYR	3.2
1	B	74	LEU	3.2
1	A	273	GLY	3.1
1	B	278	GLN	3.1
1	B	335	VAL	3.1
1	A	164	LEU	3.1
1	B	352	PRO	3.1
1	B	270	HIS	3.0
1	A	37	PHE	2.9
1	B	300	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	160	ASN	2.9
1	B	279	LEU	2.9
1	A	261	ILE	2.9
1	A	354	THR	2.9
1	B	225	ASP	2.9
1	A	73	GLN	2.8
1	B	198	HIS	2.8
1	A	219	SER	2.8
1	B	70	SER	2.8
1	A	182	ASN	2.7
1	B	186	ARG	2.7
1	A	303	LEU	2.7
1	B	283	VAL	2.6
1	B	69	ASN	2.6
1	B	263	GLY	2.6
1	A	165	GLY	2.6
1	B	282	ILE	2.6
1	A	70	SER	2.5
1	B	181	LEU	2.5
1	B	291	GLY	2.5
1	B	266	ILE	2.4
1	B	143	ILE	2.4
1	A	88	ARG	2.4
1	B	301	ASN	2.4
1	B	341	GLN	2.4
1	A	221	ASP	2.4
1	B	353	ALA	2.4
1	B	222	LYS	2.4
1	A	136	GLY	2.3
1	B	230	GLU	2.3
1	A	296	ALA	2.3
1	B	304	ILE	2.3
1	B	344	LEU	2.3
1	A	305	ILE	2.3
1	B	280	GLN	2.3
1	B	305	ILE	2.3
1	B	136	GLY	2.2
1	B	226	GLY	2.2
1	B	262	GLY	2.2
1	B	68	THR	2.2
1	A	74	LEU	2.2
1	A	135	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	223	SER	2.2
1	B	285	ASN	2.1
1	A	226	GLY	2.1
1	B	185	GLY	2.1
1	B	336	MET	2.1
1	B	340	LYS	2.1
1	A	258	TYR	2.1
1	A	311	PRO	2.1
1	B	260	GLY	2.1
1	B	78	THR	2.1
1	B	73	GLN	2.1
1	B	39	SER	2.0
1	A	227	GLU	2.0
1	A	67	ASN	2.0
1	B	348	ILE	2.0
1	A	283	VAL	2.0
1	B	284	VAL	2.0
1	B	227	GLU	2.0
1	B	315	ALA	2.0
1	B	72	ASN	2.0
1	B	168	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.