



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:45 am BST

PDB ID : 1TE0
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

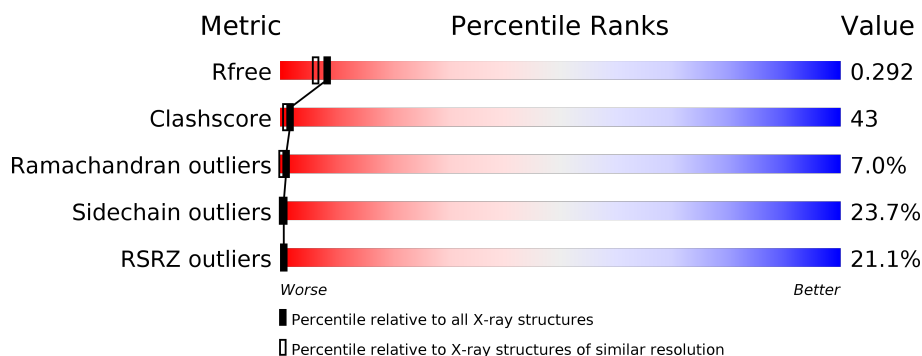
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	<div> <div>16%</div> <div> <div>47%</div> <div>29%</div> <div>16%</div> <div>7%</div> </div> </div>
1	B	318	<div> <div>26%</div> <div> <div>43%</div> <div>32%</div> <div>17%</div> <div>8%</div> </div> </div>

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

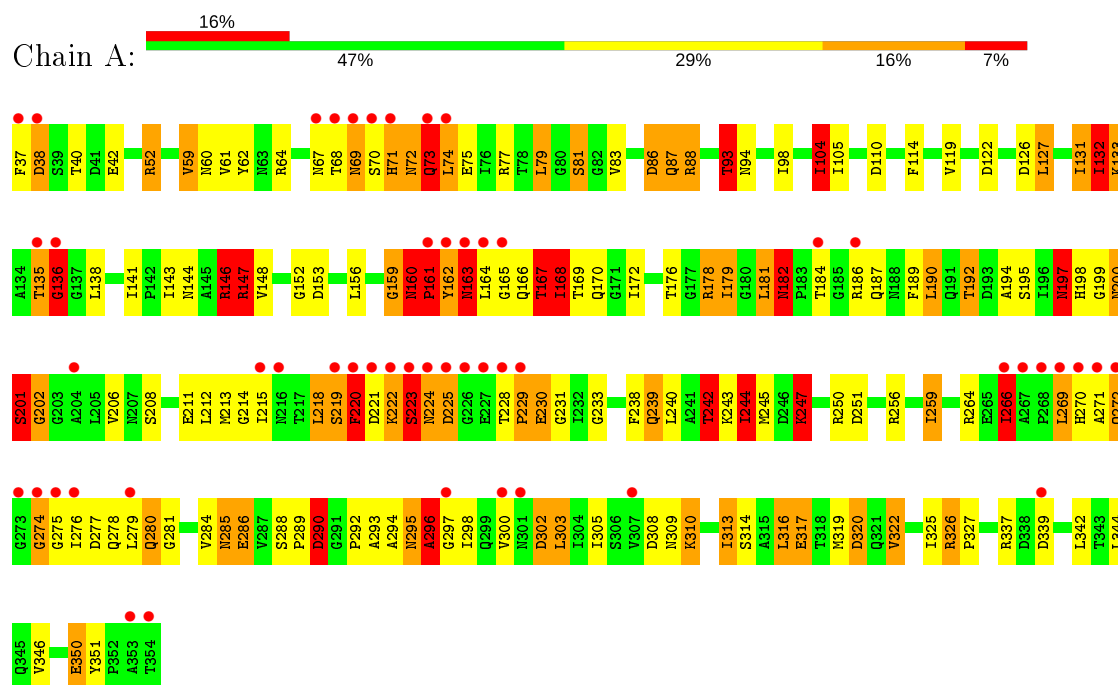
- Molecule 2 is water.

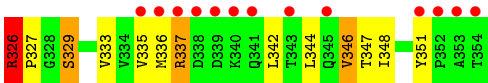
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		
2	B	77	Total	O	0	0
			77	77		

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.

• Molecule 1: Protease degS





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 32.61 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.62-2.20) 99.0 (32.61-2.20)	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 , 70.1	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	1.81	43/2362 (1.8%)	1.75	66/3216 (2.1%)
1	B	1.89	42/2362 (1.8%)	1.75	59/3216 (1.8%)
All	All	1.85	85/4724 (1.8%)	1.75	125/6432 (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	1	8
1	B	1	6
All	All	2	14

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	GLY	N-CA	11.56	1.63	1.46
1	B	90	TYR	CE2-CZ	11.29	1.53	1.38
1	A	197	ASN	CB-CG	-10.64	1.26	1.51
1	B	83	VAL	CB-CG2	10.32	1.74	1.52
1	B	219	SER	CB-OG	9.75	1.54	1.42
1	A	200	ASN	CA-CB	9.42	1.77	1.53
1	A	245	MET	SD-CE	-9.18	1.26	1.77
1	B	202	GLY	N-CA	9.02	1.59	1.46
1	B	201	SER	CB-OG	-8.80	1.30	1.42
1	B	242	THR	CB-CG2	-8.63	1.23	1.52
1	A	200	ASN	CB-CG	-8.57	1.31	1.51
1	A	59	VAL	CB-CG2	-8.50	1.35	1.52
1	B	154	VAL	CB-CG1	8.12	1.70	1.52
1	A	219	SER	CB-OG	8.10	1.52	1.42
1	B	90	TYR	CG-CD1	7.79	1.49	1.39
1	A	178	ARG	CG-CD	7.71	1.71	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	GLU	CD-OE1	-7.70	1.17	1.25
1	B	92	ILE	C-O	7.67	1.38	1.23
1	A	59	VAL	CB-CG1	7.65	1.69	1.52
1	A	219	SER	CA-CB	7.45	1.64	1.52
1	A	202	GLY	CA-C	7.35	1.63	1.51
1	B	258	TYR	CD2-CE2	7.14	1.50	1.39
1	B	39	SER	CB-OG	-7.06	1.33	1.42
1	B	202	GLY	C-O	7.06	1.34	1.23
1	A	88	ARG	N-CA	6.98	1.60	1.46
1	A	242	THR	CB-CG2	-6.96	1.29	1.52
1	B	200	ASN	CB-CG	-6.85	1.35	1.51
1	A	214	GLY	C-O	6.61	1.34	1.23
1	B	245	MET	SD-CE	-6.55	1.41	1.77
1	B	200	ASN	CA-CB	6.55	1.70	1.53
1	A	238	PHE	CD2-CE2	6.48	1.52	1.39
1	B	133	LYS	CD-CE	6.42	1.67	1.51
1	A	256	ARG	CD-NE	6.25	1.57	1.46
1	A	200	ASN	CG-OD1	6.23	1.37	1.24
1	A	208	SER	CA-CB	6.16	1.62	1.52
1	B	197	ASN	CB-CG	-6.12	1.36	1.51
1	B	52	ARG	NE-CZ	6.10	1.41	1.33
1	A	144	ASN	CB-CG	6.10	1.65	1.51
1	A	148	VAL	CB-CG2	6.08	1.65	1.52
1	B	241	ALA	CA-CB	6.07	1.65	1.52
1	B	216	ASN	N-CA	6.04	1.58	1.46
1	B	51	VAL	CB-CG2	6.01	1.65	1.52
1	B	200	ASN	CG-OD1	6.01	1.37	1.24
1	A	182	ASN	CB-CG	5.98	1.64	1.51
1	A	52	ARG	CG-CD	5.96	1.66	1.51
1	B	168	ILE	CB-CG2	-5.94	1.34	1.52
1	B	155	VAL	CB-CG1	5.94	1.65	1.52
1	B	104	ILE	CA-CB	5.89	1.68	1.54
1	A	208	SER	CB-OG	5.89	1.50	1.42
1	B	174	SER	CB-OG	5.83	1.49	1.42
1	B	219	SER	CA-CB	5.79	1.61	1.52
1	B	167	THR	CA-CB	5.73	1.68	1.53
1	A	322	VAL	CA-CB	5.67	1.66	1.54
1	A	37	PHE	N-CA	5.63	1.57	1.46
1	A	52	ARG	NE-CZ	5.61	1.40	1.33
1	A	148	VAL	N-CA	5.61	1.57	1.46
1	A	206	VAL	CA-CB	5.58	1.66	1.54
1	B	271	ALA	CA-CB	5.58	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	305	ILE	CA-CB	5.54	1.67	1.54
1	A	147	ARG	CG-CD	-5.54	1.38	1.51
1	B	247	LYS	CG-CD	-5.51	1.33	1.52
1	A	197	ASN	CA-CB	5.50	1.67	1.53
1	B	239	GLN	CG-CD	5.49	1.63	1.51
1	A	215	ILE	CB-CG2	5.44	1.69	1.52
1	A	201	SER	CA-CB	5.39	1.61	1.52
1	B	228	THR	CA-CB	5.38	1.67	1.53
1	B	174	SER	CA-CB	5.33	1.60	1.52
1	A	243	LYS	C-O	5.32	1.33	1.23
1	A	81	SER	CA-CB	5.31	1.60	1.52
1	B	47	TYR	CG-CD1	5.31	1.46	1.39
1	A	83	VAL	CB-CG2	5.30	1.64	1.52
1	A	167	THR	CA-CB	5.28	1.67	1.53
1	B	147	ARG	CD-NE	-5.27	1.37	1.46
1	B	147	ARG	CG-CD	-5.18	1.39	1.51
1	B	244	ILE	CA-CB	5.16	1.66	1.54
1	B	50	ALA	CA-CB	5.15	1.63	1.52
1	B	141	ILE	CB-CG2	5.15	1.68	1.52
1	A	83	VAL	C-O	-5.14	1.13	1.23
1	B	258	TYR	CD1-CE1	5.12	1.47	1.39
1	A	62	TYR	CD1-CE1	5.12	1.47	1.39
1	A	233	GLY	CA-C	5.10	1.60	1.51
1	A	189	PHE	CD2-CE2	5.10	1.49	1.39
1	A	146	ARG	CB-CG	5.09	1.66	1.52
1	A	152	GLY	C-O	5.07	1.31	1.23
1	B	84	ILE	CB-CG2	5.00	1.68	1.52

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	SER	C-N-CA	-15.63	89.47	122.30
1	A	201	SER	C-N-CA	-14.89	91.03	122.30
1	B	251	ASP	CB-CG-OD2	14.58	131.42	118.30
1	A	178	ARG	NE-CZ-NH2	-14.29	113.15	120.30
1	A	147	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	A	247	LYS	CD-CE-NZ	-11.43	85.41	111.70
1	A	302	ASP	CB-CG-OD2	11.24	128.42	118.30
1	A	146	ARG	NE-CZ-NH1	-11.14	114.73	120.30
1	B	190	LEU	CA-CB-CG	11.09	140.80	115.30
1	A	251	ASP	CB-CG-OD2	11.05	128.25	118.30
1	A	38	ASP	CB-CG-OD2	10.57	127.81	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	ARG	NE-CZ-NH1	-10.07	115.27	120.30
1	B	38	ASP	CB-CG-OD2	9.50	126.85	118.30
1	B	126	ASP	CB-CG-OD2	9.49	126.84	118.30
1	A	79	LEU	CA-CB-CG	9.40	136.93	115.30
1	B	201	SER	CA-CB-OG	-9.22	86.32	111.20
1	A	308	ASP	CB-CG-OD2	8.97	126.37	118.30
1	A	190	LEU	CA-CB-CG	8.61	135.10	115.30
1	A	302	ASP	CB-CG-OD1	-8.49	110.66	118.30
1	A	225	ASP	N-CA-C	8.24	133.26	111.00
1	B	303	LEU	CA-CB-CG	8.15	134.04	115.30
1	A	147	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	178	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	126	ASP	CB-CG-OD2	8.04	125.54	118.30
1	B	302	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	161	PRO	N-CA-C	7.64	131.96	112.10
1	B	74	LEU	CA-CB-CG	7.63	132.85	115.30
1	A	87	GLN	O-C-N	-7.62	110.50	122.70
1	B	225	ASP	N-CA-C	7.55	131.39	111.00
1	A	88	ARG	CB-CA-C	-7.51	95.39	110.40
1	B	253	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	B	326	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	B	161	PRO	N-CA-C	7.36	131.22	112.10
1	B	326	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	B	147	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	200	ASN	CB-CG-OD1	-7.28	107.04	121.60
1	B	193	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	244	ILE	CA-CB-CG2	7.17	125.25	110.90
1	B	192	THR	CA-CB-CG2	7.17	122.44	112.40
1	B	253	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	B	112	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	B	201	SER	O-C-N	-6.87	111.52	123.20
1	B	122	ASP	CB-CG-OD2	6.86	124.48	118.30
1	B	342	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	B	197	ASN	CB-CA-C	-6.81	96.78	110.40
1	B	132	ILE	CA-CB-CG2	6.79	124.47	110.90
1	A	86	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	151	ILE	CG1-CB-CG2	-6.71	96.64	111.40
1	A	146	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	201	SER	O-C-N	-6.60	111.97	123.20
1	A	132	ILE	CA-CB-CG2	6.59	124.08	110.90
1	B	59	VAL	CG1-CB-CG2	6.54	121.37	110.90
1	A	178	ARG	CG-CD-NE	-6.53	98.08	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	THR	N-CA-C	6.51	128.58	111.00
1	B	217	THR	CA-CB-CG2	-6.48	103.33	112.40
1	A	344	LEU	CA-CB-CG	-6.44	100.48	115.30
1	B	200	ASN	CB-CG-OD1	-6.40	108.80	121.60
1	B	104	ILE	CA-CB-CG2	6.33	123.56	110.90
1	A	242	THR	N-CA-CB	-6.32	98.29	110.30
1	A	87	GLN	C-N-CA	-6.32	105.91	121.70
1	B	244	ILE	CA-CB-CG2	6.30	123.50	110.90
1	A	197	ASN	CB-CA-C	-6.29	97.81	110.40
1	A	110	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	200	ASN	CA-CB-CG	-6.17	99.82	113.40
1	B	244	ILE	CB-CG1-CD1	-6.11	96.79	113.90
1	A	127	LEU	CB-CG-CD1	-6.06	100.69	111.00
1	B	190	LEU	CB-CG-CD1	6.05	121.29	111.00
1	B	87	GLN	N-CA-C	-6.04	94.70	111.00
1	B	74	LEU	N-CA-C	6.03	127.28	111.00
1	A	342	LEU	CB-CG-CD2	-5.99	100.82	111.00
1	A	244	ILE	CB-CG1-CD1	-5.97	97.18	113.90
1	A	250	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	41	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	222	LYS	N-CA-C	5.88	126.89	111.00
1	A	308	ASP	OD1-CG-OD2	-5.86	112.17	123.30
1	B	79	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	181	LEU	CA-CB-CG	5.85	128.75	115.30
1	B	59	VAL	CA-CB-CG1	5.83	119.64	110.90
1	B	167	THR	OG1-CB-CG2	-5.83	96.60	110.00
1	B	124	LEU	CA-CB-CG	-5.77	102.04	115.30
1	B	192	THR	CB-CA-C	-5.75	96.06	111.60
1	B	93	THR	CB-CA-C	-5.75	96.07	111.60
1	B	200	ASN	CA-CB-CG	-5.75	100.75	113.40
1	A	222	LYS	N-CA-C	5.74	126.51	111.00
1	B	251	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	A	74	LEU	CB-CG-CD1	5.72	120.73	111.00
1	B	242	THR	CA-CB-CG2	5.71	120.40	112.40
1	A	224	ASN	C-N-CA	5.66	135.84	121.70
1	B	308	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	71	HIS	N-CA-C	5.64	126.22	111.00
1	A	221	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	168	ILE	N-CA-C	5.60	126.11	111.00
1	B	77	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	316	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	286	GLU	N-CA-C	-5.49	96.17	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	B	166	GLN	N-CA-C	5.44	125.69	111.00
1	A	93	THR	CB-CA-C	-5.43	96.93	111.60
1	A	122	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	153	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	59	VAL	N-CA-CB	-5.35	99.73	111.50
1	A	220	PHE	N-CA-C	5.33	125.38	111.00
1	A	350	GLU	N-CA-CB	5.30	120.13	110.60
1	B	227	GLU	N-CA-C	5.28	125.27	111.00
1	A	339	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	277	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	104	ILE	CB-CA-C	5.24	122.08	111.60
1	A	156	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	192	THR	CA-CB-OG1	5.21	119.93	109.00
1	A	285	ASN	CB-CA-C	-5.20	100.00	110.40
1	A	192	THR	CA-CB-CG2	5.20	119.68	112.40
1	B	64	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	296	ALA	N-CA-C	5.17	124.97	111.00
1	B	53	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	59	VAL	CA-CB-CG1	5.15	118.63	110.90
1	A	201	SER	N-CA-CB	5.14	118.21	110.50
1	A	320	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	168	ILE	N-CA-C	5.12	124.82	111.00
1	B	258	TYR	CB-CA-C	-5.12	100.17	110.40
1	B	166	GLN	CB-CA-C	-5.11	100.18	110.40
1	A	201	SER	CA-C-N	5.08	126.36	116.20
1	B	201	SER	CA-C-N	5.07	126.33	116.20
1	B	86	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	71	HIS	N-CA-C	5.01	124.54	111.00
1	A	290	ASP	CB-CG-OD2	5.00	122.80	118.30

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	176	2
1	B	2333	0	2356	231	1
2	A	86	0	0	43	1
2	B	77	0	0	41	2
All	All	4829	0	4712	407	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 43.

All (407) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:A:160:ASN:N	1.40	1.13
1:A:146:ARG:HH11	1:A:146:ARG:HG2	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:HA	1:A:200:ASN:OD1	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:CG	1:B:146:ARG:HH11	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
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: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:B:146:ARG:HG2	1:B:146:ARG:HH11	0.83	0.96
1:A:337:ARG:HH11	1:A:337:ARG:HG3	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:38:ASP:O	1:B:38:ASP:CG	2.07	0.93
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:HD22	1:A:69:ASN:H	1.02	0.93
1:B:135:THR:HA	2:B:372:HOH:O	1.68	0.92
1:A:200:ASN:CA	1:A:200:ASN:CG	2.38	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:A:146:ARG:HG2	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:O	1:A:38:ASP:OD1	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:165:GLY:HA2	2:B:426:HOH:O	1.74	0.87
1:B:67:ASN:ND2	1:B:69:ASN:ND2	2.23	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
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:B:38:ASP:OD1	1:B:38:ASP:O	1.97	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: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:162:TYR:HA	2:A:407:HOH:O	1.80	0.82
1:A:87:GLN:O	1:A:88:ARG:CG	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:104:ILE:C	1:B:104:ILE:HD12	2.04	0.78
1:B:146:ARG:CG	1:B:146:ARG:NH1	2.34	0.78
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:CG1	1:B:83:VAL:CG2	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:160:ASN:O	1:B:165:GLY:O	2.04	0.76
1:B:72:ASN:O	1:B:73:GLN:HB2	1.83	0.76
1:A:302:ASP:CG	1:A:337:ARG:HH12	1.88	0.75
1:B:186:ARG:HH11	1:B:186:ARG:HG3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:N	1:A:69:ASN:HD22	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:182:ASN:ND2	1:A:182:ASN:N	2.41	0.69
1:A:168:ILE:CB	2:A:410:HOH:O	2.41	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
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: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	0.67
1:B:135:THR:HG22	2:B:372:HOH:O	1.94	0.66
1:B:119:VAL:HG23	1:B:131:ILE:HG22	1.76	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: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:198:HIS:HB3	1:A:225:ASP:CB	2.26	0.65
1:A:38:ASP:HA	2:A:370:HOH:O	1.96	0.65
1:A:146:ARG:NH1	1:A:146:ARG:CG	2.46	0.65
1:A:229:PRO:O	1:A:230:GLU:CB	2.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:O	1:A:72:ASN:CB	2.45	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:A:71:HIS:C	1:A:72:ASN:HD22	2.01	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:135:THR:O	1:B:136:GLY:C	2.36	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:186:ARG:CG	1:B:186:ARG:HH11	2.12	0.62
1:B:285:ASN:O	1:B:300:VAL:HG23	1.98	0.62
1:A:269:LEU:H	1:A:269:LEU:HD23	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:HD22	1:B:182:ASN:N	1.98	0.62
1:A:119:VAL:HG23	1:A:131:ILE:HG22	1.81	0.62
1:B:104:ILE:CD1	1:B:104:ILE:C	2.67	0.62
1:B:60:ASN:OD1	1:B:160:ASN:CG	2.37	0.62
1:B:298:ILE:CG1	1:B:344:LEU:HD12	2.28	0.62
1:B:186:ARG:NH1	1:B:186:ARG:HG3	2.07	0.62
1:A:104:ILE:HD12	1:A:104:ILE:C	2.21	0.61
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:200:ASN:CB	1:A:200:ASN:C	2.66	0.61
1:A:135:THR:O	1:A:136:GLY:C	2.36	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:B:287:VAL:O	1:B:288:SER:C	2.40	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:71:HIS:C	1:B:72:ASN:HD22	2.05	0.59
1:A:114:PHE:HB2	1:A:132:ILE:HG12	1.84	0.59
1:A:337:ARG:NH1	1:A:337:ARG:HG3	2.03	0.59
1:B:104:ILE:CD1	1:B:105:ILE:N	2.66	0.59
1:B:289:PRO:O	1:B:290:ASP:C	2.41	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:298:ILE:HG12	1:B:344:LEU:CD1	2.31	0.58
1:B:94:ASN:HD21	1:B:201:SER:CB	2.10	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:B:313:ILE:HG23	1:B:313:ILE:O	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:295:ASN:N	1:B:295:ASN:ND2	2.40	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
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:HE21	1:A:73:GLN:HA	1.72	0.55
1:A:182:ASN:H	1:A:182:ASN:ND2	1.99	0.55
1:B:87:GLN:HA	2:B:381:HOH:O	2.00	0.55
1:A:73:GLN:NE2	1:A:73:GLN:HA	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:A:201:SER:O	1:A:202:GLY:C	2.30	0.54
1:B:48:ASN:HD21	1:B:52:ARG:HE	1.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:160:ASN:C	1:B:165:GLY:O	2.45	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:B:324:GLU:CG	2:B:385:HOH:O	2.56	0.53
1:B:178:ARG:HB2	1:B:188:ASN:HA	1.89	0.53
1:B:86:ASP:OD1	1:B:88:ARG:HB2	2.09	0.53
1:A:284:VAL:HB	1:A:300:VAL:O	2.08	0.53
1:A:160:ASN:CB	1:A:161:PRO:CD	2.72	0.52
1:A:67:ASN:HB2	1:A:69:ASN:ND2	2.24	0.52
1:A:181:LEU:CD1	1:A:247:LYS:HZ1	2.23	0.52
1:A:69:ASN:N	1:A:69:ASN:ND2	2.49	0.52
1:A:285:ASN:O	1:A:300:VAL:HG23	2.10	0.52
1:A:86:ASP:OD1	1:A:88:ARG:HB2	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
1:B:337:ARG:CG	1:B:337:ARG:HH11	1.97	0.52
1:B:59:VAL:HG22	1:B:108:LEU:HD22	1.92	0.52
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:A:168:ILE:HG12	1:A:169:THR:N	2.24	0.51
1:B:247:LYS:CE	2:B:361:HOH:O	2.40	0.51
1:A:293:ALA:O	1:A:297:GLY:O	2.28	0.50
1:A:141:ILE:HG12	1:A:212:LEU:HD13	1.93	0.50
1:B:159:GLY:C	1:B:160:ASN:ND2	2.65	0.50
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: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:197:ASN:HB3	1:A:199:GLY:H	1.77	0.48
1:A:64:ARG:NH1	2:A:393:HOH:O	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:HD13	1:B:105:ILE:N	2.28	0.48
1:A:182:ASN:CG	1:A:320:ASP:OD1	2.52	0.48
1:B:69:ASN:ND2	1:B:69:ASN:N	2.47	0.48
1:B:179:ILE:CG2	1:B:179:ILE:O	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:192:THR:CG2	1:B:194:ALA:H	2.18	0.48
1:B:67:ASN:HB3	1:B:72:ASN:HA	1.95	0.48
1:B:229:PRO:O	1:B:230:GLU:CB	2.61	0.48
1:A:319:MET:HE2	2:A:425:HOH:O	2.02	0.47
1:B:220:PHE:N	1:B:220:PHE:CD1	2.82	0.47
1:B:220:PHE:N	1:B:220:PHE:HD1	2.13	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:86:ASP:C	1:B:87:GLN:O	2.49	0.47
1:B:337:ARG:NH1	1:B:337:ARG:CG	2.62	0.47
1:B:94:ASN:HD21	1:B:201:SER:C	2.18	0.47
1:B:266:ILE:HG12	1:B:283:VAL:HG22	1.95	0.47
1:A:133:LYS:CE	2:A:375:HOH:O	2.44	0.47
1:B:69:ASN:O	1:B:70:SER:C	2.53	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:A:294:ALA:O	1:A:297:GLY:HA2	2.16	0.46
1:A:219:SER:C	2:A:435:HOH:O	2.42	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:160:ASN:CB	1:A:161:PRO:HD2	2.43	0.45
1:A:52:ARG:HD3	2:A:396:HOH:O	2.17	0.45
1:B:185:GLY:HA3	1:B:188:ASN:HD22	1.81	0.45
1:B:69:ASN:O	1:B:70:SER:O	2.34	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:324:GLU:HG3	2:B:385:HOH:O	2.16	0.45
1:B:298:ILE:CG1	1:B:344:LEU:CD1	2.92	0.45
1:B:59:VAL:CG2	1:B:108:LEU:HD22	2.47	0.45
1:A:81:SER:O	1:A:93:THR:CG2	2.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG21	1:A:313:ILE:HD13	1.56	0.44
1:B:293:ALA:C	1:B:295:ASN:O	2.56	0.44
1:B:326:ARG:HH11	1:B:326:ARG:HG3	1.81	0.44
1:A:166:GLN:CG	2:A:406:HOH:O	2.37	0.44
1:A:61:VAL:HG13	1:A:104:ILE:CD1	2.48	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
1:B:326:ARG:NH1	1:B:326:ARG:CG	2.77	0.44
1:B:302:ASP:CB	1:B:337:ARG:NH1	2.80	0.44
1:A:266:ILE:HD11	1:A:281:GLY:HA3	2.00	0.44
1:A:302:ASP:C	1:A:302:ASP:OD1	2.56	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:HD3	1:B:253:ARG:HH11	1.57	0.44
1:A:228:THR:O	1:A:229:PRO:O	2.36	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:HD23	1:B:269:LEU:H	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:A:182:ASN:CG	1:A:182:ASN:O	2.55	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:289:PRO:O	1:A:290:ASP:C	2.56	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:A:60:ASN:OD1	1:A:160:ASN:CG	2.57	0.42
1:B:160:ASN:O	1:B:166:GLN:HA	2.18	0.42
1:B:305:ILE:HA	1:B:305:ILE:HD12	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:A:98:ILE:C	1:A:98:ILE:HD12	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLN:NE2	1:B:73:GLN:HA	2.34	0.42
1:B:313:ILE:HG22	1:B:314:SER:CB	2.46	0.42
1:B:178:ARG:HD3	1:B:178:ARG:HH11	1.65	0.42
1:B:265:GLU:HA	1:B:281:GLY:O	2.20	0.42
1:B:201:SER:O	1:B:202:GLY:C	2.33	0.42
1:B:168:ILE:HG21	1:B:168:ILE:HD12	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:A:295:ASN:H	1:A:295:ASN:HD22	1.66	0.41
1:B:114:PHE:CB	1:B:132:ILE:HG12	2.50	0.41
1:A:159:GLY:C	1:A:160:ASN:ND2	2.70	0.41
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:337:ARG:CG	1:A:337:ARG:NH1	2.77	0.41
1:B:143:ILE:HD13	1:B:143:ILE:HG21	1.78	0.41
1:B:313:ILE:HD13	1:B:313:ILE:HG21	1.73	0.41
1:A:228:THR:N	1:A:229:PRO:HD2	2.36	0.41
1:A:94:ASN:HD21	1:A:201:SER:CB	2.13	0.41
1:B:214:GLY:HA2	1:B:236:ILE:O	2.20	0.41
1:B:87:GLN:O	1:B:88:ARG:CG	2.68	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:B:302:ASP:CG	1:B:337:ARG:HH12	2.24	0.40
1:B:247:LYS:NZ	2:B:361:HOH:O	2.53	0.40
1:B:87:GLN:CB	2:B:381:HOH:O	2.59	0.40
1:A:38:ASP:OD1	1:A:38:ASP:C	2.55	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 ⓘ

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%)	193 (78%)	56 (22%)	1	1
1	B	249/257 (97%)	187 (75%)	62 (25%)	0	0
All	All	498/514 (97%)	380 (76%)	118 (24%)	1	0

All (118) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75	GLU
1	A	77	ARG
1	A	93	THR
1	A	104	ILE
1	A	131	ILE
1	A	132	ILE
1	A	133	LYS
1	A	135	THR
1	A	143	ILE
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	170	GLN
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	223	SER
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	346	VAL
1	A	350	GLU
1	A	351	TYR
1	B	39	SER
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	131	ILE
1	B	132	ILE
1	B	133	LYS
1	B	135	THR
1	B	143	ILE
1	B	146	ARG
1	B	147	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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	239	GLN
1	B	242	THR
1	B	244	ILE
1	B	247	LYS
1	B	250	ARG
1	B	259	ILE
1	B	264	ARG
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	288	SER
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	337	ARG
1	B	346	VAL
1	B	351	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	182	ASN
1	A	188	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	239	GLN
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	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.







5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	1.14	51 (16%)  	33, 54, 81, 85	0
1	B	318/318 (100%)	1.47	83 (26%)  	34, 54, 81, 85	0
All	All	636/636 (100%)	1.31	134 (21%)  	33, 54, 81, 85	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	GLY	12.9
1	A	162	TYR	11.9
1	B	271	ALA	11.1
1	A	224	ASN	11.1
1	B	276	ILE	10.9
1	B	229	PRO	10.9
1	A	271	ALA	9.6
1	A	269	LEU	9.0
1	A	223	SER	8.7
1	A	268	PRO	8.6
1	B	163	ASN	8.5
1	B	164	LEU	8.5
1	A	229	PRO	8.5
1	B	184	THR	8.2
1	B	268	PRO	8.1
1	B	228	THR	8.0
1	B	273	GLY	8.0
1	B	270	HIS	7.9
1	B	162	TYR	7.9
1	B	277	ASP	7.6
1	B	183	PRO	7.6
1	A	222	LYS	7.2
1	B	354	THR	7.0
1	A	270	HIS	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	220	PHE	6.8
1	B	269	LEU	6.7
1	A	221	ASP	6.6
1	A	272	GLN	6.6
1	B	267	ALA	6.5
1	B	278	GLN	6.5
1	A	163	ASN	6.4
1	B	289	PRO	6.3
1	B	279	LEU	6.3
1	A	37	PHE	6.1
1	A	220	PHE	6.0
1	A	71	HIS	5.9
1	B	186	ARG	5.8
1	B	224	ASN	5.8
1	B	275	GLY	5.8
1	B	339	ASP	5.5
1	B	222	LYS	5.5
1	B	37	PHE	5.4
1	B	352	PRO	5.4
1	B	341	GLN	5.3
1	B	227	GLU	5.3
1	A	354	THR	5.3
1	A	186	ARG	5.3
1	B	223	SER	5.2
1	B	353	ALA	5.1
1	A	276	ILE	5.1
1	A	70	SER	4.9
1	B	298	ILE	4.9
1	B	221	ASP	4.8
1	B	272	GLN	4.8
1	A	69	ASN	4.8
1	B	226	GLY	4.8
1	A	73	GLN	4.7
1	A	267	ALA	4.7
1	B	299	GLN	4.6
1	A	273	GLY	4.5
1	A	228	THR	4.4
1	B	172	ILE	4.4
1	B	296	ALA	4.4
1	B	291	GLY	4.4
1	B	336	MET	4.4
1	B	335	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	353	ALA	4.3
1	A	161	PRO	4.1
1	B	38	ASP	4.0
1	B	171	GLY	4.0
1	B	165	GLY	3.9
1	A	300	VAL	3.9
1	A	226	GLY	3.8
1	A	135	THR	3.8
1	B	225	ASP	3.8
1	B	161	PRO	3.8
1	B	340	LYS	3.7
1	A	164	LEU	3.7
1	B	219	SER	3.6
1	A	38	ASP	3.6
1	B	258	TYR	3.5
1	B	155	VAL	3.5
1	B	351	TYR	3.5
1	A	136	GLY	3.4
1	B	266	ILE	3.4
1	A	279	LEU	3.4
1	B	154	VAL	3.3
1	B	301	ASN	3.3
1	A	227	GLU	3.3
1	B	303	LEU	3.3
1	B	345	GLN	3.2
1	A	266	ILE	3.1
1	A	274	GLY	3.1
1	A	219	SER	3.0
1	B	300	VAL	3.0
1	A	74	LEU	3.0
1	A	225	ASP	2.9
1	B	343	THR	2.9
1	A	297	GLY	2.9
1	B	194	ALA	2.9
1	B	74	LEU	2.8
1	B	264	ARG	2.8
1	B	187	GLN	2.7
1	B	338	ASP	2.7
1	B	170	GLN	2.7
1	A	307	VAL	2.7
1	B	136	GLY	2.6
1	A	215	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	280	GLN	2.6
1	B	337	ARG	2.6
1	B	156	LEU	2.6
1	B	290	ASP	2.5
1	B	146	ARG	2.5
1	A	68	THR	2.5
1	A	301	ASN	2.5
1	B	305	ILE	2.5
1	B	263	GLY	2.4
1	A	67	ASN	2.4
1	B	297	GLY	2.4
1	A	184	THR	2.4
1	B	41	ASP	2.4
1	A	275	GLY	2.4
1	A	204	ALA	2.2
1	B	169	THR	2.2
1	B	284	VAL	2.2
1	A	165	GLY	2.2
1	A	339	ASP	2.2
1	B	157	ALA	2.1
1	B	313	ILE	2.1
1	B	70	SER	2.1
1	B	193	ASP	2.1
1	A	216	ASN	2.1
1	B	66	LEU	2.0
1	B	192	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.