



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:34 PM UTC

PDB ID : 1RXX / pdb_00001rxx
Title : Structure of arginine deiminase
Authors : Galkin, A.; Kulakova, L.; Sarikaya, E.; Lim, K.; Howard, A.; Herzberg, O.;
Structure 2 Function Project (S2F)
Deposited on : 2003-12-18
Resolution : 2.45 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
Mogul : 2022.3.0, CSD as543be (2022)
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

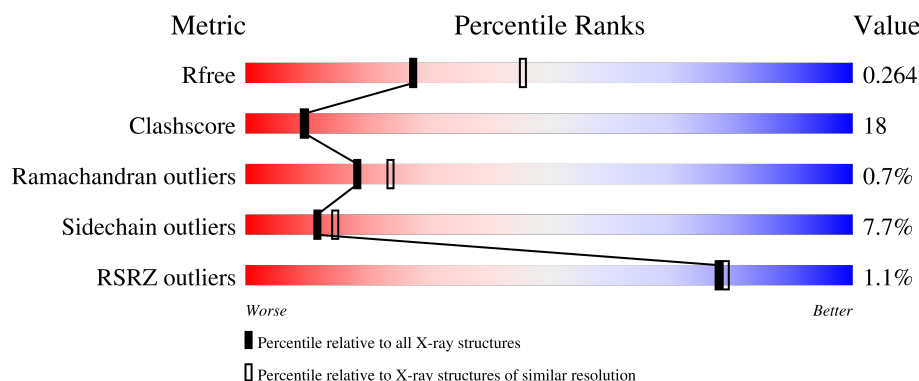
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	421	% 62% 28% 7% .
1	B	421	63% 26% 6% .
1	C	421	% 66% 27% 5% ..
1	D	421	% 62% 28% 5% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13187 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 Arginine deiminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	Se	0	0	0
			3185	2015	553	600	7	10			
1	B	404	Total	C	N	O	S	Se	0	0	0
			3160	2001	549	593	7	10			
1	C	412	Total	C	N	O	S	Se	0	0	0
			3214	2033	557	607	7	10			
1	D	402	Total	C	N	O	S	Se	0	0	0
			3136	1986	543	590	7	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P13981
A	-1	SER	-	cloning artifact	UNP P13981
A	0	HIS	-	cloning artifact	UNP P13981
A	1	MSE	-	cloning artifact	UNP P13981
A	21	MSE	MET	modified residue	UNP P13981
A	62	MSE	MET	modified residue	UNP P13981
A	72	MSE	MET	modified residue	UNP P13981
A	143	MSE	MET	modified residue	UNP P13981
A	180	MSE	MET	modified residue	UNP P13981
A	229	MSE	MET	modified residue	UNP P13981
A	240	MSE	MET	modified residue	UNP P13981
A	277	MSE	MET	modified residue	UNP P13981
A	316	MSE	MET	modified residue	UNP P13981
A	407	MSE	MET	modified residue	UNP P13981
B	-2	GLY	-	cloning artifact	UNP P13981
B	-1	SER	-	cloning artifact	UNP P13981
B	0	HIS	-	cloning artifact	UNP P13981
B	1	MSE	-	cloning artifact	UNP P13981
B	21	MSE	MET	modified residue	UNP P13981
B	62	MSE	MET	modified residue	UNP P13981
B	72	MSE	MET	modified residue	UNP P13981

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	143	MSE	MET	modified residue	UNP P13981
B	180	MSE	MET	modified residue	UNP P13981
B	229	MSE	MET	modified residue	UNP P13981
B	240	MSE	MET	modified residue	UNP P13981
B	277	MSE	MET	modified residue	UNP P13981
B	316	MSE	MET	modified residue	UNP P13981
B	407	MSE	MET	modified residue	UNP P13981
C	-2	GLY	-	cloning artifact	UNP P13981
C	-1	SER	-	cloning artifact	UNP P13981
C	0	HIS	-	cloning artifact	UNP P13981
C	1	MSE	-	cloning artifact	UNP P13981
C	21	MSE	MET	modified residue	UNP P13981
C	62	MSE	MET	modified residue	UNP P13981
C	72	MSE	MET	modified residue	UNP P13981
C	143	MSE	MET	modified residue	UNP P13981
C	180	MSE	MET	modified residue	UNP P13981
C	229	MSE	MET	modified residue	UNP P13981
C	240	MSE	MET	modified residue	UNP P13981
C	277	MSE	MET	modified residue	UNP P13981
C	316	MSE	MET	modified residue	UNP P13981
C	407	MSE	MET	modified residue	UNP P13981
D	-2	GLY	-	cloning artifact	UNP P13981
D	-1	SER	-	cloning artifact	UNP P13981
D	0	HIS	-	cloning artifact	UNP P13981
D	1	MSE	-	cloning artifact	UNP P13981
D	21	MSE	MET	modified residue	UNP P13981
D	62	MSE	MET	modified residue	UNP P13981
D	72	MSE	MET	modified residue	UNP P13981
D	143	MSE	MET	modified residue	UNP P13981
D	180	MSE	MET	modified residue	UNP P13981
D	229	MSE	MET	modified residue	UNP P13981
D	240	MSE	MET	modified residue	UNP P13981
D	277	MSE	MET	modified residue	UNP P13981
D	316	MSE	MET	modified residue	UNP P13981
D	407	MSE	MET	modified residue	UNP P13981

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	113	Total O 113 113	0	0
2	B	147	Total O 147 147	0	0

Continued on next page...

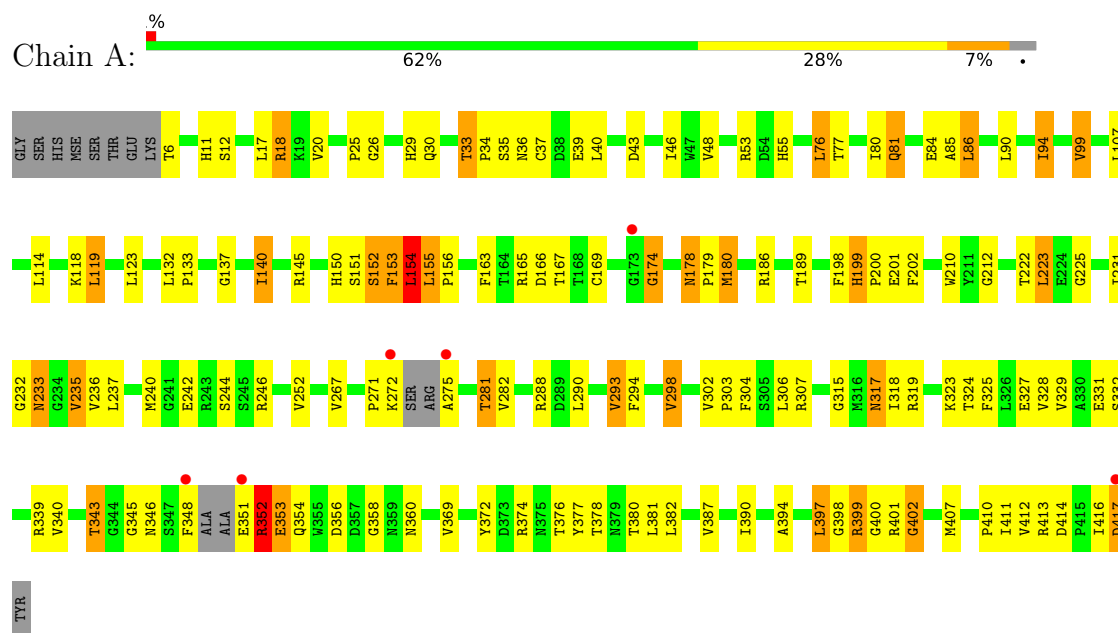
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	144	Total 144	O 144	0	0
2	D	88	Total 88	O 88	0	0

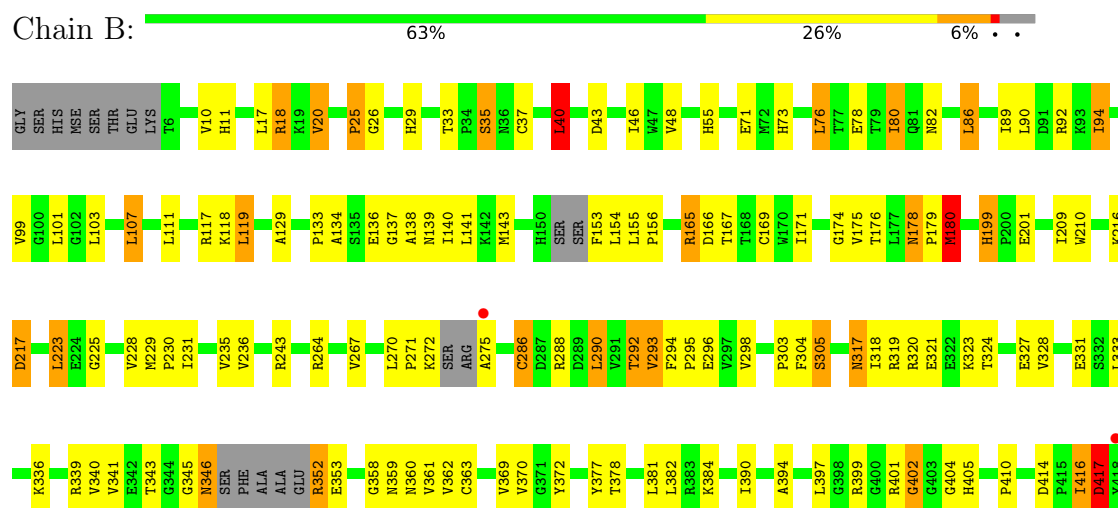
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Arginine deiminase



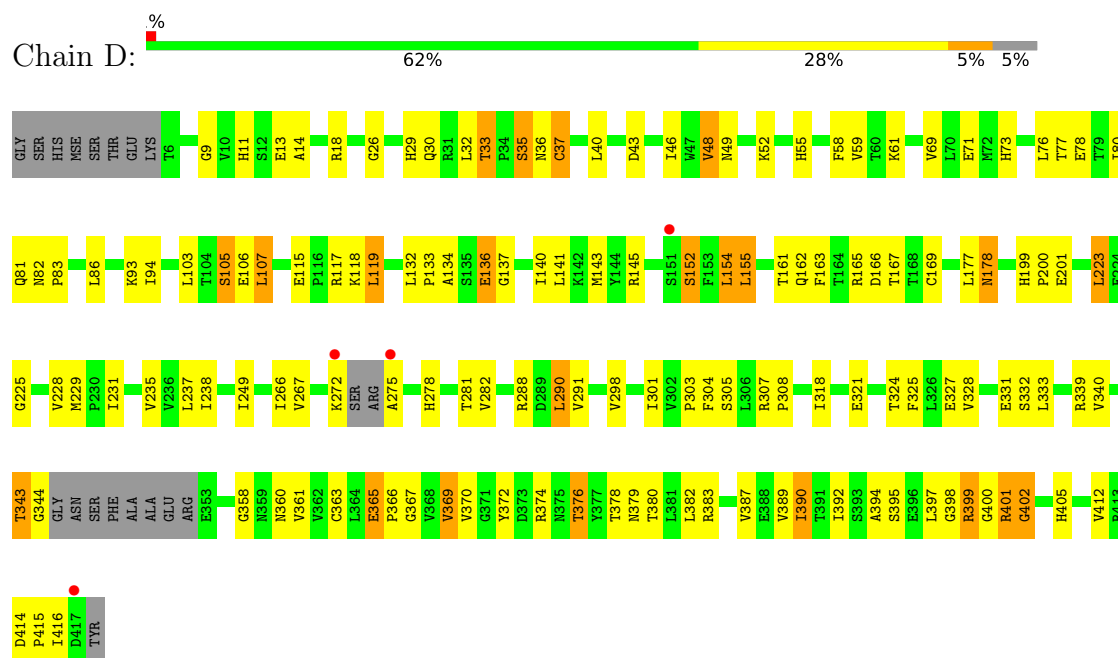
• Molecule 1: Arginine deiminase



• Molecule 1: Arginine deiminase



• Molecule 1: Arginine deiminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.90Å 114.90Å 300.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 20.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.45) 99.7 (20.00-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 2.44Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.264 0.200 , 0.264	Depositor DCC
R_{free} test set	3802 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13187	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.68% 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	0.87	1/3242 (0.0%)	1.27	38/4379 (0.9%)
1	B	0.89	2/3216 (0.1%)	1.22	28/4342 (0.6%)
1	C	0.85	0/3273	1.29	33/4422 (0.7%)
1	D	0.78	0/3192	1.22	19/4313 (0.4%)
All	All	0.85	3/12923 (0.0%)	1.25	118/17456 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	MSE	SE-CE	-14.56	1.51	1.95
1	B	370	VAL	CA-CB	-5.61	1.47	1.54
1	A	252	VAL	CA-CB	5.16	1.60	1.54

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	SER	N-CA-C	11.54	135.38	110.80
1	C	346	ASN	N-CA-C	11.29	127.68	109.85
1	D	154	LEU	N-CA-C	-10.17	100.19	111.07
1	B	167	THR	N-CA-C	10.11	124.97	112.23
1	A	43	ASP	N-CA-C	9.78	121.94	111.28
1	C	166	ASP	N-CA-C	9.58	121.33	111.07
1	C	400	GLY	N-CA-C	-9.29	91.63	110.69
1	D	166	ASP	N-CA-C	9.08	120.78	111.07
1	C	178	ASN	N-CA-C	8.75	122.36	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	GLY	N-CA-C	8.68	127.80	115.30
1	A	167	THR	N-CA-C	8.38	123.28	112.89
1	C	274	ARG	N-CA-C	-8.33	102.71	113.12
1	C	167	THR	N-CA-C	8.26	123.13	112.89
1	D	365	GLU	N-CA-C	-8.13	100.91	108.22
1	D	43	ASP	N-CA-C	7.91	120.90	111.33
1	A	48	VAL	N-CA-C	7.60	117.71	110.42
1	A	178	ASN	N-CA-C	7.58	119.46	109.83
1	D	389	VAL	N-CA-C	7.39	118.31	107.37
1	A	411	ILE	N-CA-C	-7.32	105.27	111.56
1	D	340	VAL	N-CA-C	7.18	118.16	108.11
1	C	292	THR	N-CA-C	-7.16	99.93	110.52
1	B	48	VAL	N-CA-C	7.03	117.74	110.36
1	B	43	ASP	N-CA-C	6.93	118.48	111.07
1	D	178	ASN	N-CA-C	6.82	121.52	109.58
1	C	218	HIS	N-CA-C	6.80	121.24	113.15
1	A	174	GLY	N-CA-C	-6.78	100.35	110.38
1	A	166	ASP	N-CA-C	6.77	118.32	111.07
1	D	37	CYS	N-CA-C	6.72	119.18	111.11
1	A	153	PHE	N-CA-C	6.70	119.06	108.67
1	C	365	GLU	N-CA-C	-6.67	102.13	108.13
1	A	340	VAL	N-CA-C	6.61	117.64	108.12
1	D	228	VAL	N-CA-C	6.50	117.22	107.80
1	B	178	ASN	CA-C-N	6.45	127.90	119.84
1	B	178	ASN	C-N-CA	6.45	127.90	119.84
1	A	387	VAL	N-CA-C	6.42	117.54	108.36
1	B	217	ASP	N-CA-C	6.42	121.37	112.45
1	A	352	ARG	N-CA-C	6.41	119.72	108.75
1	B	390	ILE	CB-CA-C	-6.40	102.44	111.21
1	B	228	VAL	N-CA-C	6.40	117.51	108.36
1	B	294	PHE	CA-C-N	6.33	127.75	119.84
1	B	294	PHE	C-N-CA	6.33	127.75	119.84
1	D	167	THR	N-CA-C	6.32	120.73	112.89
1	C	340	VAL	N-CA-C	6.31	117.11	107.77
1	C	177	LEU	N-CA-C	-6.29	96.05	107.75
1	D	11	HIS	N-CA-C	6.29	121.10	113.17
1	A	81	GLN	N-CA-C	-6.22	105.18	112.89
1	A	339	ARG	N-CA-C	-6.21	100.40	110.20
1	D	376	THR	N-CA-C	6.19	118.82	111.33
1	A	156	PRO	N-CA-C	6.15	116.37	110.47
1	C	309	ASP	CA-C-N	6.13	126.31	119.32
1	C	309	ASP	C-N-CA	6.13	126.31	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	365	GLU	N-CA-CB	-6.10	105.54	111.27
1	C	156	PRO	CA-C-N	6.03	126.00	120.03
1	C	156	PRO	C-N-CA	6.03	126.00	120.03
1	C	81	GLN	N-CA-C	-6.01	105.95	113.28
1	B	166	ASP	N-CA-C	6.00	117.49	111.07
1	A	155	LEU	CA-C-N	-6.00	115.28	119.66
1	A	155	LEU	C-N-CA	-6.00	115.28	119.66
1	C	48	VAL	N-CA-C	5.99	116.45	110.23
1	A	199	HIS	CA-C-N	5.97	127.31	119.84
1	A	199	HIS	C-N-CA	5.97	127.31	119.84
1	B	339	ARG	N-CA-C	-5.95	100.80	110.20
1	B	11	HIS	N-CA-C	5.94	120.66	113.17
1	D	390	ILE	CB-CA-C	-5.94	102.91	111.34
1	A	180	MSE	CG-SE-CE	-5.92	85.90	98.92
1	A	202	PHE	N-CA-C	5.91	120.87	113.43
1	B	178	ASN	N-CA-C	5.90	119.90	109.58
1	A	294	PHE	N-CA-C	-5.85	96.89	109.01
1	C	133	PRO	N-CA-C	-5.85	101.97	110.80
1	A	387	VAL	CB-CA-C	-5.82	102.93	110.84
1	A	11	HIS	N-CA-C	5.81	120.38	112.88
1	C	228	VAL	N-CA-C	5.76	116.15	107.80
1	C	346	ASN	CA-C-N	5.71	132.45	121.54
1	C	346	ASN	C-N-CA	5.71	132.45	121.54
1	B	25	PRO	N-CA-C	-5.61	102.30	111.21
1	B	360	ASN	N-CA-C	5.60	119.41	112.58
1	C	316	MSE	N-CA-C	5.58	117.45	109.14
1	D	374	ARG	N-CA-C	5.55	118.10	111.71
1	D	282	VAL	CB-CA-C	-5.55	104.83	110.93
1	B	340	VAL	N-CA-C	5.54	116.09	108.12
1	A	298	VAL	N-CA-C	5.52	116.25	110.62
1	A	132	LEU	CA-C-N	-5.44	114.35	119.85
1	A	132	LEU	C-N-CA	-5.44	114.35	119.85
1	A	94	ILE	N-CA-C	5.44	114.57	106.85
1	A	212	GLY	N-CA-C	5.44	118.38	112.29
1	C	179	PRO	N-CA-C	-5.43	101.72	110.74
1	A	390	ILE	N-CA-C	-5.38	101.78	108.89
1	C	25	PRO	N-CA-C	-5.37	103.01	111.34
1	A	25	PRO	N-CA-C	-5.36	102.68	111.21
1	A	233	ASN	N-CA-C	-5.36	104.74	111.92
1	D	399	ARG	N-CA-C	-5.36	106.44	112.87
1	B	40	LEU	N-CA-C	-5.35	106.34	112.92
1	C	273	SER	N-CA-C	-5.35	100.99	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	PRO	N-CA-C	-5.34	102.89	111.38
1	C	43	ASP	N-CA-C	5.32	116.88	111.14
1	B	243	ARG	N-CA-C	5.31	120.77	113.97
1	C	156	PRO	O-C-N	5.29	123.64	121.15
1	B	270	LEU	CA-C-N	5.28	125.18	119.85
1	B	270	LEU	C-N-CA	5.28	125.18	119.85
1	B	199	HIS	CA-C-N	5.25	124.70	119.24
1	B	199	HIS	C-N-CA	5.25	124.70	119.24
1	D	177	LEU	N-CA-C	-5.24	96.82	107.41
1	D	48	VAL	N-CA-C	5.24	115.68	110.23
1	C	37	CYS	N-CA-C	5.22	117.39	111.02
1	C	297	VAL	N-CA-C	5.22	115.88	110.82
1	B	229	MSE	CA-C-N	-5.18	113.36	119.84
1	B	229	MSE	C-N-CA	-5.18	113.36	119.84
1	A	154	LEU	N-CA-C	-5.16	105.55	111.07
1	C	20	VAL	CB-CA-C	-5.14	101.51	110.71
1	A	381	LEU	N-CA-C	-5.07	105.94	111.82
1	B	286	CYS	N-CA-C	-5.07	108.13	114.56
1	D	35	SER	N-CA-C	5.07	119.17	112.89
1	A	235	VAL	N-CA-C	5.04	117.09	109.12
1	B	292	THR	N-CA-C	-5.04	102.61	110.42
1	B	94	ILE	N-CA-C	5.04	114.73	106.72
1	A	252	VAL	N-CA-C	-5.01	105.82	110.53
1	A	412	VAL	CB-CA-C	-5.00	104.48	110.99
1	C	298	VAL	N-CA-C	5.00	115.72	110.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	144	TYR	Sidechain
1	C	348	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3185	0	3161	124	0
1	B	3160	0	3139	117	0
1	C	3214	0	3186	102	0
1	D	3136	0	3119	109	0
2	A	113	0	0	15	0
2	B	147	0	0	16	0
2	C	144	0	0	20	0
2	D	88	0	0	13	0
All	All	13187	0	12605	444	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (444) 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:352:ARG:HG3	1:B:352:ARG:HH11	1.13	1.11
1:A:343:THR:HG21	1:A:358:GLY:H	1.15	1.08
1:B:343:THR:HG21	1:B:358:GLY:H	1.21	1.04
1:D:343:THR:HG21	1:D:358:GLY:H	1.20	1.02
1:B:363:CYS:HB2	2:B:517:HOH:O	1.61	1.01
1:A:346:ASN:HB3	1:B:35:SER:HB3	1.45	0.98
1:A:352:ARG:HB3	2:A:436:HOH:O	1.60	0.98
1:A:306:LEU:HD13	1:A:318:ILE:HG12	1.49	0.94
1:C:399:ARG:HA	1:C:399:ARG:CZ	1.98	0.94
1:C:33:THR:HG22	1:C:36:ASN:H	1.37	0.90
1:B:361:VAL:HA	2:B:523:HOH:O	1.71	0.89
1:A:178:ASN:HB2	1:A:180:MSE:HE1	1.56	0.88
1:A:293:VAL:HG22	1:A:298:VAL:HG21	1.55	0.88
1:B:352:ARG:HG3	1:B:352:ARG:NH1	1.86	0.87
1:C:343:THR:HB	2:C:534:HOH:O	1.73	0.87
1:A:180:MSE:SE	2:A:515:HOH:O	2.43	0.86
1:C:398:GLY:HA2	2:C:551:HOH:O	1.74	0.85
1:C:130:ASP:HB2	2:C:545:HOH:O	1.78	0.82
1:B:199:HIS:CD2	1:B:201:GLU:H	1.97	0.81
1:B:343:THR:CG2	1:B:358:GLY:H	1.92	0.81
1:B:352:ARG:N	2:B:516:HOH:O	2.13	0.81
1:A:343:THR:HG21	1:A:358:GLY:N	1.96	0.81
1:C:343:THR:HG21	1:C:358:GLY:H	1.45	0.80
1:D:343:THR:CG2	1:D:358:GLY:H	1.94	0.80
1:A:343:THR:CG2	1:A:358:GLY:H	1.94	0.79
1:D:33:THR:HG22	1:D:36:ASN:H	1.47	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:HIS:CD2	1:D:201:GLU:H	2.01	0.79
1:A:271:PRO:O	1:A:272:LYS:HB3	1.82	0.78
1:B:199:HIS:HD2	1:B:201:GLU:H	1.28	0.78
1:A:307:ARG:HD2	2:A:514:HOH:O	1.84	0.77
1:C:348:PHE:O	1:C:349:ALA:HB2	1.83	0.77
1:A:376:THR:O	1:A:380:THR:HG23	1.85	0.77
1:D:46:ILE:HG22	1:D:399:ARG:HD2	1.66	0.77
1:B:17:LEU:HD11	1:B:20:VAL:HG13	1.65	0.76
1:A:240:MSE:HE2	1:A:246:ARG:CA	2.17	0.75
1:A:145:ARG:HD3	1:A:152:SER:HB3	1.70	0.73
1:A:17:LEU:HD11	1:A:20:VAL:CG1	2.19	0.73
1:B:343:THR:HG23	1:B:378:THR:OG1	1.87	0.73
1:A:272:LYS:HZ1	1:A:275:ALA:N	1.87	0.73
1:C:402:GLY:HA3	2:C:551:HOH:O	1.87	0.73
1:A:352:ARG:HG2	1:A:377:TYR:CD1	2.24	0.73
1:A:352:ARG:HD3	1:A:353:GLU:H	1.54	0.72
1:C:240:MSE:HE2	1:C:246:ARG:HA	1.71	0.72
1:D:267:VAL:HB	1:D:304:PHE:HB2	1.71	0.72
1:B:17:LEU:HD21	1:B:20:VAL:HG11	1.71	0.72
1:D:343:THR:HG21	1:D:358:GLY:N	2.01	0.72
1:A:324:THR:O	1:A:328:VAL:HG23	1.90	0.71
1:D:71:GLU:OE2	1:D:73:HIS:HB2	1.90	0.71
1:D:199:HIS:HD2	1:D:201:GLU:H	1.37	0.71
1:A:240:MSE:HE2	1:A:246:ARG:HA	1.73	0.70
1:A:352:ARG:HG2	1:A:377:TYR:CE1	2.26	0.70
1:B:55:HIS:HD2	2:B:521:HOH:O	1.72	0.70
1:D:103:LEU:HD13	1:D:154:LEU:CD1	2.22	0.70
1:B:137:GLY:O	1:B:140:ILE:HG12	1.92	0.70
1:C:33:THR:HG22	1:C:36:ASN:N	2.06	0.70
1:D:237:LEU:HD23	1:D:266:ILE:HB	1.73	0.69
1:D:136:GLU:CD	1:D:137:GLY:H	2.00	0.69
1:A:343:THR:HG23	1:A:378:THR:OG1	1.92	0.69
1:A:345:GLY:HA3	1:A:348:PHE:CE2	2.28	0.69
1:B:103:LEU:CD1	1:B:141:LEU:HD11	2.22	0.69
1:D:49:ASN:HB3	2:D:477:HOH:O	1.91	0.68
1:B:343:THR:HG21	1:B:358:GLY:N	2.02	0.68
1:B:363:CYS:CB	2:B:517:HOH:O	2.29	0.68
1:B:352:ARG:HD3	2:B:519:HOH:O	1.94	0.68
1:D:358:GLY:HA3	1:D:378:THR:HG21	1.75	0.67
1:D:343:THR:HG23	1:D:378:THR:OG1	1.95	0.67
1:B:17:LEU:HD11	1:B:20:VAL:CG1	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.59	0.67
1:D:343:THR:HG22	1:D:344:GLY:H	1.60	0.66
1:D:288:ARG:HG2	1:D:416:ILE:HG21	1.76	0.66
1:B:165:ARG:O	1:B:225:GLY:HA3	1.94	0.66
1:A:18:ARG:HE	1:A:414:ASP:CG	2.03	0.66
1:A:178:ASN:HB3	1:A:223:LEU:O	1.96	0.66
1:A:331:GLU:HB2	2:A:512:HOH:O	1.96	0.66
1:B:317:ASN:HD21	1:B:319:ARG:HD3	1.58	0.66
1:B:359:ASN:HB3	2:B:543:HOH:O	1.96	0.66
1:C:358:GLY:HA3	1:C:378:THR:HG21	1.76	0.66
1:B:293:VAL:HG22	1:B:298:VAL:HG21	1.78	0.65
1:A:17:LEU:HD21	1:A:20:VAL:HG11	1.77	0.65
1:D:80:ILE:HD12	1:D:119:LEU:HD13	1.79	0.65
1:A:33:THR:HG22	1:A:36:ASN:H	1.62	0.65
1:D:324:THR:OG1	1:D:327:GLU:HG3	1.97	0.65
1:A:178:ASN:O	1:A:180:MSE:HE2	1.96	0.65
1:C:360:ASN:OD1	1:C:403:GLY:HA3	1.97	0.65
1:C:106:GLU:HG2	2:C:541:HOH:O	1.96	0.64
1:D:30:GLN:NE2	2:D:490:HOH:O	2.27	0.64
1:D:77:THR:HG21	1:D:117:ARG:HD2	1.79	0.64
1:A:325:PHE:O	1:A:329:VAL:HG23	1.98	0.64
1:A:178:ASN:O	1:A:180:MSE:CE	2.47	0.63
1:D:376:THR:O	1:D:380:THR:HG23	1.97	0.63
1:D:48:VAL:HG12	1:D:52:LYS:HE2	1.79	0.63
1:A:145:ARG:HD3	1:A:152:SER:CB	2.28	0.63
1:A:165:ARG:O	1:A:225:GLY:HA3	1.98	0.63
1:B:103:LEU:HD11	1:B:141:LEU:HD11	1.81	0.63
1:B:416:ILE:HG22	1:B:417:ASP:N	2.14	0.62
1:C:295:PRO:O	1:C:299:LYS:HG2	2.00	0.62
1:A:53:ARG:HD3	1:C:64:GLU:OE1	2.00	0.61
1:A:17:LEU:HD11	1:A:20:VAL:HG13	1.82	0.61
1:A:20:VAL:HG12	1:A:410:PRO:HA	1.82	0.61
1:A:186:ARG:HG2	2:A:440:HOH:O	2.00	0.61
1:B:199:HIS:HD2	1:B:201:GLU:N	1.98	0.61
1:A:240:MSE:CE	1:A:246:ARG:HA	2.30	0.61
1:B:80:ILE:HD11	1:B:89:ILE:HD12	1.81	0.61
1:B:288:ARG:HH22	1:B:417:ASP:HB3	1.66	0.61
1:C:153:PHE:HB2	2:C:533:HOH:O	2.01	0.60
1:D:361:VAL:HB	1:D:369:VAL:HG13	1.83	0.60
1:C:286:CYS:HA	2:C:539:HOH:O	2.01	0.60
1:D:29:HIS:CD2	1:D:29:HIS:H	2.18	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASN:ND2	1:B:319:ARG:HD3	2.16	0.60
1:C:150:HIS:CE1	2:C:535:HOH:O	2.54	0.60
1:D:137:GLY:O	1:D:140:ILE:HG12	2.01	0.60
1:B:264:ARG:HD2	1:B:305:SER:OG	2.01	0.60
1:C:286:CYS:HB2	1:C:290:LEU:HD13	1.83	0.60
1:D:33:THR:HG23	1:D:35:SER:H	1.66	0.60
1:A:84:GLU:HG2	1:A:198:PHE:CE1	2.36	0.60
1:D:324:THR:O	1:D:328:VAL:HG23	2.01	0.60
1:C:363:CYS:SG	2:C:539:HOH:O	2.57	0.59
1:D:372:TYR:CG	1:D:394:ALA:HB2	2.36	0.59
1:A:35:SER:OG	1:B:346:ASN:HB2	2.01	0.59
1:A:80:ILE:HD12	1:A:119:LEU:HD13	1.85	0.59
1:A:222:THR:O	1:A:244:SER:HA	2.03	0.58
1:A:240:MSE:HE2	1:A:246:ARG:CB	2.34	0.58
1:A:328:VAL:HA	1:A:331:GLU:HG2	1.85	0.58
1:C:165:ARG:O	1:C:225:GLY:HA3	2.03	0.58
1:B:119:LEU:O	1:B:119:LEU:HD22	2.03	0.58
1:B:156:PRO:HD2	2:B:440:HOH:O	2.03	0.58
1:B:180:MSE:HE2	1:B:180:MSE:HA	1.84	0.58
1:C:145:ARG:HD3	1:C:152:SER:HB3	1.86	0.58
1:C:363:CYS:HB2	2:C:539:HOH:O	2.03	0.58
1:D:106:GLU:HG2	2:D:451:HOH:O	2.04	0.58
1:A:55:HIS:HD2	2:A:433:HOH:O	1.87	0.57
1:A:240:MSE:HE2	1:A:246:ARG:HB3	1.85	0.57
1:B:323:LYS:HB3	1:B:327:GLU:OE1	2.04	0.57
1:C:33:THR:HG23	1:C:35:SER:H	1.69	0.57
1:D:59:VAL:HG13	1:D:69:VAL:HG11	1.86	0.57
1:D:398:GLY:C	1:D:400:GLY:H	2.11	0.57
1:A:398:GLY:C	1:A:400:GLY:H	2.12	0.57
1:B:352:ARG:NH1	2:B:520:HOH:O	2.38	0.57
1:D:107:LEU:HD11	1:D:155:LEU:HD22	1.87	0.57
1:A:84:GLU:HG2	1:A:198:PHE:HE1	1.69	0.56
1:C:193:THR:HG21	1:C:214:PRO:HG3	1.87	0.56
1:D:115:GLU:HG2	2:D:506:HOH:O	2.05	0.56
1:C:103:LEU:HD13	1:C:154:LEU:CD1	2.35	0.56
1:D:94:ILE:HD13	1:D:107:LEU:HD13	1.88	0.56
1:A:151:SER:HB2	2:A:510:HOH:O	2.04	0.56
1:B:178:ASN:HB2	1:B:180:MSE:HE1	1.86	0.56
1:A:77:THR:O	1:A:81:GLN:HG3	2.07	0.55
1:A:118:LYS:HD3	2:A:495:HOH:O	2.06	0.55
1:B:103:LEU:HD13	1:B:141:LEU:HD11	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:VAL:HB	1:B:304:PHE:HB2	1.88	0.55
1:A:345:GLY:HA3	1:A:348:PHE:HE2	1.69	0.55
1:D:55:HIS:O	1:D:58:PHE:HB3	2.06	0.55
1:A:18:ARG:HH11	1:A:18:ARG:CG	2.20	0.54
1:A:153:PHE:N	2:A:472:HOH:O	2.34	0.54
1:B:78:GLU:OE1	1:B:199:HIS:HE1	1.89	0.54
1:B:303:PRO:HG2	1:B:321:GLU:HB2	1.88	0.54
1:C:178:ASN:HB3	1:C:223:LEU:O	2.07	0.54
1:D:33:THR:HG22	1:D:36:ASN:N	2.19	0.54
1:D:33:THR:CG2	1:D:35:SER:H	2.20	0.54
1:B:404:GLY:HA3	2:B:523:HOH:O	2.06	0.54
1:D:118:LYS:HD3	2:D:506:HOH:O	2.07	0.54
1:D:372:TYR:CD2	1:D:394:ALA:HB2	2.43	0.54
1:C:33:THR:CG2	1:C:35:SER:H	2.20	0.54
1:A:99:VAL:HG22	1:A:154:LEU:HD12	1.90	0.54
1:C:343:THR:HG23	1:C:378:THR:OG1	2.07	0.54
1:D:145:ARG:HD3	1:D:152:SER:OG	2.08	0.54
1:B:169:CYS:HB2	1:B:176:THR:OG1	2.07	0.54
1:B:286:CYS:HB2	1:B:290:LEU:HD13	1.90	0.54
1:D:303:PRO:HB2	1:D:321:GLU:HB2	1.89	0.54
1:D:398:GLY:C	1:D:400:GLY:N	2.63	0.54
1:B:359:ASN:CB	2:B:543:HOH:O	2.55	0.54
1:C:293:VAL:HG13	1:C:298:VAL:HG21	1.90	0.54
1:D:141:LEU:HD11	1:D:154:LEU:HD13	1.90	0.54
1:D:367:GLY:O	1:D:387:VAL:HG13	2.07	0.54
1:B:174:GLY:HA3	1:B:210:TRP:CE2	2.43	0.53
1:C:398:GLY:O	1:C:399:ARG:C	2.51	0.53
1:C:26:GLY:H	1:C:29:HIS:CD2	2.27	0.53
1:B:296:GLU:HB2	2:B:546:HOH:O	2.08	0.53
1:A:267:VAL:HB	1:A:304:PHE:HB2	1.90	0.53
1:C:71:GLU:OE2	1:C:73:HIS:HB2	2.08	0.53
1:A:12:SER:O	1:A:413:ARG:HD2	2.09	0.53
1:C:103:LEU:CD1	1:C:141:LEU:HD11	2.38	0.53
1:C:361:VAL:HG21	1:C:369:VAL:HG21	1.91	0.53
1:C:376:THR:O	1:C:380:THR:HG23	2.09	0.53
1:D:165:ARG:O	1:D:225:GLY:HA3	2.08	0.53
1:C:363:CYS:CB	2:C:539:HOH:O	2.55	0.53
1:D:29:HIS:CD2	1:D:29:HIS:N	2.77	0.53
1:D:231:ILE:HD12	1:D:333:LEU:HD21	1.91	0.53
1:A:174:GLY:HA3	1:A:210:TRP:NE1	2.23	0.52
1:B:17:LEU:HD21	1:B:20:VAL:CG1	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:HE2	1:A:275:ALA:O	2.09	0.52
1:B:18:ARG:HE	1:B:414:ASP:CG	2.17	0.52
1:B:46:ILE:HG22	1:B:399:ARG:HD2	1.92	0.52
1:B:293:VAL:O	1:B:295:PRO:HD3	2.09	0.52
1:A:26:GLY:H	1:A:29:HIS:CD2	2.27	0.52
1:B:352:ARG:N	1:B:352:ARG:HD3	2.25	0.52
1:D:343:THR:HG22	1:D:344:GLY:N	2.24	0.52
1:C:399:ARG:HA	1:C:399:ARG:NE	2.24	0.52
1:C:18:ARG:NE	1:C:414:ASP:OD2	2.43	0.51
1:B:94:ILE:HD13	1:B:107:LEU:HD13	1.92	0.51
1:D:278:HIS:O	1:D:281:THR:HB	2.10	0.51
1:C:166:ASP:HB3	1:C:180:MSE:HE1	1.91	0.51
1:D:165:ARG:CZ	1:D:405:HIS:CE1	2.93	0.51
1:A:240:MSE:CE	1:A:246:ARG:HB3	2.40	0.51
1:C:63:ARG:NH1	2:C:554:HOH:O	2.42	0.51
1:A:33:THR:CG2	1:A:35:SER:H	2.23	0.51
1:B:352:ARG:N	1:B:352:ARG:CD	2.74	0.51
1:A:199:HIS:CD2	1:A:201:GLU:H	2.29	0.51
1:C:26:GLY:H	1:C:29:HIS:HD2	1.59	0.51
1:C:343:THR:HG22	1:C:344:GLY:N	2.24	0.51
1:A:119:LEU:O	1:A:123:LEU:HG	2.11	0.50
1:A:345:GLY:HA3	1:A:348:PHE:CD2	2.45	0.50
1:A:374:ARG:NE	2:A:429:HOH:O	2.30	0.50
1:D:103:LEU:HD13	1:D:154:LEU:HD11	1.92	0.50
1:D:272:LYS:HZ3	1:D:275:ALA:N	2.08	0.50
1:B:178:ASN:HB3	1:B:223:LEU:O	2.11	0.50
1:C:278:HIS:O	1:C:281:THR:HB	2.11	0.50
1:C:293:VAL:O	1:C:295:PRO:HD3	2.11	0.50
1:B:372:TYR:CG	1:B:394:ALA:HB2	2.46	0.50
1:D:165:ARG:NH2	2:D:465:HOH:O	2.42	0.50
1:A:174:GLY:HA3	1:A:210:TRP:CE2	2.47	0.50
1:B:352:ARG:HB3	2:B:527:HOH:O	2.10	0.49
1:A:235:VAL:HG12	1:A:236:VAL:N	2.27	0.49
1:B:71:GLU:OE1	1:B:73:HIS:N	2.45	0.49
1:D:344:GLY:C	2:D:474:HOH:O	2.55	0.49
1:A:114:LEU:HD22	1:A:118:LYS:HE3	1.94	0.49
1:D:93:LYS:HD2	2:D:444:HOH:O	2.12	0.49
1:C:163:PHE:CE1	1:C:402:GLY:HA2	2.48	0.49
1:D:105:SER:HB3	2:D:493:HOH:O	2.11	0.49
1:D:298:VAL:HA	1:D:301:ILE:HD12	1.95	0.49
1:C:235:VAL:HG12	1:C:236:VAL:N	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:VAL:HG13	1:C:298:VAL:CG2	2.43	0.48
1:C:359:ASN:ND2	2:C:534:HOH:O	2.46	0.48
1:D:288:ARG:NH1	1:D:366:PRO:HB3	2.28	0.48
1:D:401:ARG:O	1:D:402:GLY:O	2.32	0.48
1:B:82:ASN:OD1	1:B:82:ASN:C	2.56	0.48
1:B:286:CYS:HA	2:B:517:HOH:O	2.12	0.48
1:C:169:CYS:SG	1:C:225:GLY:HA2	2.53	0.48
1:C:235:VAL:HG11	1:C:266:ILE:HD12	1.96	0.48
1:A:26:GLY:H	1:A:29:HIS:HD2	1.60	0.48
1:A:151:SER:CB	2:A:510:HOH:O	2.60	0.48
1:B:352:ARG:CB	2:B:527:HOH:O	2.61	0.48
1:A:281:THR:HG22	1:A:282:VAL:HG13	1.95	0.48
1:B:231:ILE:HD12	1:B:333:LEU:HD21	1.96	0.48
1:A:288:ARG:HG3	1:A:416:ILE:HG21	1.96	0.48
1:C:343:THR:CG2	1:C:378:THR:OG1	2.62	0.48
1:D:298:VAL:HA	1:D:301:ILE:CD1	2.44	0.48
1:D:414:ASP:HB3	1:D:415:PRO:HD2	1.95	0.48
1:A:288:ARG:NH1	1:A:416:ILE:HG23	2.29	0.48
1:B:292:THR:HA	1:B:341:VAL:O	2.14	0.48
1:C:23:CYS:HB3	1:C:161:THR:O	2.14	0.48
1:D:331:GLU:C	1:D:333:LEU:N	2.71	0.48
1:C:285:PHE:HA	1:C:291:VAL:HG12	1.96	0.47
1:D:394:ALA:O	1:D:395:SER:C	2.57	0.47
1:A:137:GLY:O	1:A:140:ILE:HG12	2.15	0.47
1:C:324:THR:O	1:C:328:VAL:HG23	2.13	0.47
1:C:343:THR:C	2:C:534:HOH:O	2.55	0.47
1:D:82:ASN:OD1	1:D:82:ASN:C	2.55	0.47
1:B:94:ILE:HD11	1:B:111:LEU:HD12	1.96	0.47
1:C:343:THR:O	2:C:534:HOH:O	2.20	0.47
1:A:80:ILE:HD12	1:A:119:LEU:CD1	2.44	0.47
1:D:94:ILE:CD1	1:D:107:LEU:HD13	2.45	0.47
1:D:13:GLU:OE1	1:D:229:MSE:HG2	2.15	0.47
1:B:416:ILE:CG2	1:B:417:ASP:N	2.77	0.47
1:C:394:ALA:HB1	1:C:398:GLY:HA3	1.97	0.47
1:C:399:ARG:HA	1:C:399:ARG:NH1	2.29	0.47
1:D:307:ARG:HB3	1:D:308:PRO:HD2	1.97	0.47
1:A:76:LEU:O	1:A:80:ILE:HG12	2.14	0.47
1:A:178:ASN:HA	1:A:179:PRO:HD3	1.74	0.47
1:B:20:VAL:HG12	1:B:410:PRO:HA	1.96	0.47
1:D:169:CYS:SG	1:D:225:GLY:HA2	2.55	0.47
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:MSE:CE	1:A:246:ARG:CB	2.93	0.46
1:C:17:LEU:HD11	1:C:20:VAL:HG13	1.97	0.46
1:B:26:GLY:H	1:B:29:HIS:HD2	1.63	0.46
1:C:99:VAL:HG12	1:C:103:LEU:HB2	1.96	0.46
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.79	0.46
1:B:216:LYS:CG	1:B:217:ASP:N	2.78	0.46
1:B:324:THR:O	1:B:328:VAL:HG23	2.15	0.46
1:B:345:GLY:O	1:B:346:ASN:C	2.58	0.46
1:D:14:ALA:HB3	1:D:416:ILE:HD11	1.96	0.46
1:A:417:ASP:OD2	1:A:417:ASP:C	2.57	0.46
1:C:76:LEU:O	1:C:80:ILE:HG12	2.15	0.46
1:C:165:ARG:NH2	2:C:478:HOH:O	2.48	0.46
1:B:80:ILE:CD1	1:B:89:ILE:HD12	2.45	0.46
1:B:352:ARG:HH11	1:B:352:ARG:CG	2.01	0.46
1:C:361:VAL:CG2	1:C:369:VAL:HG21	2.46	0.46
1:D:288:ARG:NH1	2:D:494:HOH:O	2.48	0.46
1:A:346:ASN:HA	1:B:33:THR:HB	1.97	0.46
1:B:86:LEU:HD22	1:B:90:LEU:HG	1.98	0.46
1:B:103:LEU:HD13	1:B:154:LEU:CD1	2.46	0.46
1:D:9:GLY:O	1:D:412:VAL:HA	2.16	0.46
1:B:76:LEU:HD22	1:B:80:ILE:HD13	1.97	0.45
1:C:356:ASP:HB2	1:C:375:ASN:OD1	2.16	0.45
1:D:61:LYS:HD3	1:D:390:ILE:CG2	2.46	0.45
1:A:90:LEU:HD22	1:A:94:ILE:HD12	1.98	0.45
1:B:235:VAL:HG12	1:B:236:VAL:N	2.31	0.45
1:D:290:LEU:HD23	1:D:339:ARG:HB2	1.99	0.45
1:A:352:ARG:HG2	1:A:377:TYR:CZ	2.51	0.45
1:D:77:THR:O	1:D:81:GLN:HG3	2.16	0.45
1:A:163:PHE:CE1	1:A:402:GLY:HA2	2.51	0.45
1:D:107:LEU:HD23	1:D:132:LEU:HD21	1.99	0.45
1:A:352:ARG:HG2	1:A:377:TYR:CG	2.51	0.45
1:C:348:PHE:O	1:C:349:ALA:CB	2.51	0.45
1:A:30:GLN:NE2	2:A:489:HOH:O	2.48	0.45
1:C:90:LEU:HD22	1:C:94:ILE:HD12	1.99	0.45
1:C:222:THR:O	1:C:244:SER:HA	2.17	0.45
1:D:33:THR:CG2	1:D:35:SER:N	2.80	0.45
1:C:18:ARG:HE	1:C:414:ASP:CG	2.25	0.45
1:B:363:CYS:SG	2:B:517:HOH:O	2.61	0.44
1:D:163:PHE:CE1	1:D:402:GLY:HA2	2.53	0.44
1:C:86:LEU:HD22	1:C:90:LEU:CD1	2.47	0.44
1:C:103:LEU:HD11	1:C:141:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:LEU:HD23	1:C:301:ILE:HG12	1.99	0.44
1:D:401:ARG:O	1:D:401:ARG:HD2	2.16	0.44
1:D:29:HIS:CE1	1:D:162:GLN:HE21	2.34	0.44
1:B:320:ARG:HH11	1:B:320:ARG:HG2	1.82	0.44
1:C:231:ILE:HD13	1:C:237:LEU:HD21	1.99	0.44
1:A:36:ASN:O	1:A:39:GLU:HG2	2.18	0.44
1:B:140:ILE:O	1:B:143:MSE:HB2	2.17	0.44
1:B:352:ARG:O	1:B:353:GLU:C	2.60	0.44
1:D:318:ILE:HG23	1:D:318:ILE:O	2.17	0.44
1:B:40:LEU:HD12	1:B:40:LEU:HA	1.83	0.44
1:C:145:ARG:HD3	1:C:152:SER:CB	2.47	0.44
1:D:290:LEU:HD22	1:D:291:VAL:N	2.32	0.44
1:A:317:ASN:CG	1:A:318:ILE:N	2.76	0.44
1:B:169:CYS:O	1:B:175:VAL:HA	2.16	0.44
1:D:29:HIS:HA	1:D:32:LEU:HG	1.99	0.44
1:D:392:ILE:HB	2:D:438:HOH:O	2.18	0.44
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.83	0.43
1:C:86:LEU:HD22	1:C:90:LEU:HG	1.99	0.43
1:C:160:ASN:HB3	1:C:185:ARG:NH2	2.33	0.43
1:C:295:PRO:O	1:C:296:GLU:C	2.61	0.43
1:A:231:ILE:HG21	1:A:237:LEU:CD1	2.48	0.43
1:C:36:ASN:O	1:C:39:GLU:HG2	2.19	0.43
1:D:18:ARG:HE	1:D:414:ASP:CG	2.26	0.43
1:D:235:VAL:HG21	1:D:332:SER:HB2	1.99	0.43
1:A:33:THR:HG23	1:B:346:ASN:CA	2.49	0.43
1:A:33:THR:HG23	1:B:346:ASN:HA	1.99	0.43
1:C:153:PHE:CB	2:C:533:HOH:O	2.65	0.43
1:C:372:TYR:CG	1:C:394:ALA:HB2	2.53	0.43
1:D:290:LEU:HD23	1:D:339:ARG:CB	2.49	0.43
1:D:383:ARG:HH11	1:D:383:ARG:HD2	1.69	0.43
1:A:55:HIS:HE1	2:A:425:HOH:O	2.02	0.43
1:B:180:MSE:HE2	1:B:180:MSE:CA	2.48	0.43
1:A:306:LEU:CD1	1:A:318:ILE:HG12	2.34	0.43
1:C:77:THR:O	1:C:81:GLN:HG3	2.19	0.43
1:D:140:ILE:HA	1:D:143:MSE:HE2	1.99	0.43
1:C:235:VAL:CG1	1:C:266:ILE:HD12	2.49	0.43
1:D:82:ASN:HA	1:D:83:PRO:HD3	1.87	0.43
1:D:370:VAL:HG22	1:D:390:ILE:HB	2.01	0.43
1:C:140:ILE:O	1:C:140:ILE:HG13	2.15	0.43
1:A:145:ARG:HD3	1:A:152:SER:OG	2.19	0.43
1:B:94:ILE:CD1	1:B:107:LEU:HD13	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:LEU:HD22	1:C:418:TYR:CE2	2.53	0.43
1:D:107:LEU:HD11	1:D:155:LEU:CD2	2.48	0.43
1:D:288:ARG:HG2	1:D:416:ILE:CG2	2.44	0.43
1:A:86:LEU:HD22	1:A:90:LEU:HG	2.01	0.43
1:B:137:GLY:O	1:B:138:ALA:C	2.61	0.43
1:B:343:THR:CG2	1:B:378:THR:OG1	2.62	0.43
1:C:394:ALA:O	1:C:395:SER:C	2.61	0.43
1:A:180:MSE:HE3	1:A:189:THR:OG1	2.19	0.42
1:B:377:TYR:CZ	1:B:381:LEU:HD11	2.54	0.42
1:D:141:LEU:HD11	1:D:154:LEU:CD1	2.50	0.42
1:D:237:LEU:CD2	1:D:266:ILE:HB	2.46	0.42
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.93	0.42
1:B:101:LEU:HA	1:B:101:LEU:HD23	1.77	0.42
1:C:213:ASP:HA	1:C:214:PRO:HD2	1.89	0.42
1:A:242:GLU:HG2	2:A:454:HOH:O	2.18	0.42
1:B:129:ALA:HA	1:B:154:LEU:HD21	2.01	0.42
1:C:373:ASP:HB3	2:C:549:HOH:O	2.19	0.42
1:D:26:GLY:H	1:D:29:HIS:CD2	2.37	0.42
1:D:238:ILE:HG21	1:D:249:ILE:HG12	2.01	0.42
1:A:374:ARG:NH2	2:A:429:HOH:O	2.48	0.42
1:C:29:HIS:CD2	1:C:29:HIS:H	2.36	0.42
1:D:303:PRO:HG3	1:D:325:PHE:HA	2.01	0.42
1:B:358:GLY:HA3	1:B:378:THR:HG21	2.01	0.42
1:B:372:TYR:CD2	1:B:394:ALA:HB2	2.55	0.42
1:C:111:LEU:HD22	1:C:119:LEU:CD2	2.50	0.42
1:C:398:GLY:O	1:C:400:GLY:N	2.52	0.42
1:A:372:TYR:CG	1:A:394:ALA:HB2	2.55	0.42
1:D:78:GLU:OE1	1:D:199:HIS:HE1	2.02	0.42
1:D:331:GLU:C	1:D:333:LEU:H	2.26	0.42
1:B:71:GLU:OE1	1:B:73:HIS:HB2	2.20	0.42
1:B:133:PRO:O	1:B:134:ALA:C	2.63	0.42
1:C:175:VAL:HG22	1:C:176:THR:N	2.35	0.42
1:D:288:ARG:HD3	2:D:494:HOH:O	2.19	0.42
1:A:328:VAL:O	1:A:331:GLU:HG3	2.20	0.42
1:D:133:PRO:O	1:D:134:ALA:C	2.63	0.42
1:C:29:HIS:CD2	1:C:29:HIS:N	2.88	0.42
1:A:33:THR:HG22	1:A:35:SER:N	2.34	0.41
1:B:92:ARG:HH11	1:B:92:ARG:HG3	1.85	0.41
1:C:103:LEU:HD13	1:C:141:LEU:HD11	2.02	0.41
1:B:18:ARG:NE	1:B:414:ASP:OD2	2.54	0.41
1:B:90:LEU:HD22	1:B:94:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLY:H	1:B:29:HIS:CD2	2.38	0.41
1:B:136:GLU:O	1:B:139:ASN:HB2	2.20	0.41
1:C:350:ALA:CB	2:C:540:HOH:O	2.68	0.41
1:D:365:GLU:O	1:D:366:PRO:C	2.63	0.41
1:B:272:LYS:HE3	1:B:275:ALA:HB3	2.02	0.41
1:D:361:VAL:HG22	2:D:429:HOH:O	2.20	0.41
1:A:232:GLY:O	1:A:233:ASN:HB3	2.20	0.41
1:A:352:ARG:HD3	1:A:353:GLU:N	2.30	0.41
1:A:17:LEU:HD21	1:A:20:VAL:CG1	2.49	0.41
1:A:398:GLY:C	1:A:400:GLY:N	2.78	0.41
1:A:85:ALA:HB2	1:A:198:PHE:CG	2.56	0.41
1:A:140:ILE:HG12	1:A:140:ILE:H	1.73	0.41
1:B:401:ARG:O	1:B:402:GLY:O	2.39	0.41
1:D:379:ASN:O	1:D:383:ARG:HG3	2.20	0.41
1:A:34:PRO:HD2	1:B:346:ASN:HB3	2.01	0.41
1:B:178:ASN:HA	1:B:179:PRO:HD2	1.82	0.41
1:D:178:ASN:HB3	1:D:223:LEU:O	2.20	0.41
1:A:33:THR:HG23	1:B:346:ASN:CB	2.50	0.41
1:A:169:CYS:SG	1:A:225:GLY:HA2	2.61	0.41
1:A:271:PRO:O	1:A:272:LYS:CB	2.60	0.41
1:A:323:LYS:HB3	1:A:327:GLU:OE1	2.20	0.41
1:B:10:VAL:HG12	1:B:230:PRO:HG2	2.03	0.41
1:B:165:ARG:HD2	1:B:405:HIS:O	2.21	0.41
1:B:362:VAL:HG13	1:B:362:VAL:O	2.21	0.41
1:C:119:LEU:O	1:C:123:LEU:HG	2.21	0.41
1:C:235:VAL:CG1	1:C:236:VAL:N	2.84	0.41
1:C:343:THR:CG2	1:C:358:GLY:H	2.23	0.41
1:C:383:ARG:HA	1:C:387:VAL:O	2.21	0.41
1:D:33:THR:HG22	1:D:35:SER:N	2.36	0.41
1:A:46:ILE:HG22	1:A:399:ARG:HD2	2.02	0.41
1:A:397:LEU:HG	1:A:407:MSE:SE	2.71	0.40
1:B:174:GLY:HA3	1:B:210:TRP:NE1	2.35	0.40
1:C:416:ILE:HD11	1:C:418:TYR:CZ	2.56	0.40
1:B:271:PRO:O	1:B:272:LYS:HB2	2.21	0.40
1:C:279:LEU:HA	1:C:279:LEU:HD12	1.86	0.40
1:A:302:VAL:HA	1:A:303:PRO:HD3	1.95	0.40
1:A:356:ASP:OD1	1:A:356:ASP:C	2.64	0.40
1:B:318:ILE:O	1:B:319:ARG:HD2	2.21	0.40
1:A:235:VAL:CG1	1:A:236:VAL:N	2.85	0.40
1:A:331:GLU:HG3	1:A:332:SER:N	2.36	0.40
1:B:99:VAL:HG12	1:B:103:LEU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ARG:NH2	1:B:417:ASP:HB3	2.34	0.40
1:C:64:GLU:HG2	2:C:468:HOH:O	2.20	0.40
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.90	0.40
1:D:199:HIS:HD2	1:D:201:GLU:N	2.11	0.40
1:A:199:HIS:HD2	1:A:201:GLU:H	1.69	0.40
1:A:401:ARG:O	1:A:402:GLY:O	2.39	0.40
1:B:153:PHE:O	1:B:154:LEU:C	2.65	0.40
1:D:343:THR:CG2	1:D:378:THR:OG1	2.66	0.40

There are no symmetry-related clashes.

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	402/421 (96%)	381 (95%)	18 (4%)	3 (1%)	18	24
1	B	396/421 (94%)	373 (94%)	21 (5%)	2 (0%)	24	32
1	C	408/421 (97%)	385 (94%)	18 (4%)	5 (1%)	10	11
1	D	396/421 (94%)	371 (94%)	23 (6%)	2 (0%)	24	32
All	All	1602/1684 (95%)	1510 (94%)	80 (5%)	12 (1%)	18	24

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	402	GLY
1	C	347	SER
1	C	402	GLY
1	D	152	SER
1	A	402	GLY
1	C	350	ALA
1	C	399	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	402	GLY
1	B	417	ASP
1	A	353	GLU
1	C	349	ALA
1	A	399	ARG

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	347/346 (100%)	316 (91%)	31 (9%)	9	10
1	B	343/346 (99%)	311 (91%)	32 (9%)	8	9
1	C	349/346 (101%)	328 (94%)	21 (6%)	17	26
1	D	342/346 (99%)	320 (94%)	22 (6%)	16	22
All	All	1381/1384 (100%)	1275 (92%)	106 (8%)	12	15

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	18	ARG
1	A	33	THR
1	A	37	CYS
1	A	40	LEU
1	A	76	LEU
1	A	86	LEU
1	A	99	VAL
1	A	107	LEU
1	A	119	LEU
1	A	140	ILE
1	A	150	HIS
1	A	152	SER
1	A	154	LEU
1	A	155	LEU
1	A	200	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	223	LEU
1	A	281	THR
1	A	290	LEU
1	A	293	VAL
1	A	317	ASN
1	A	319	ARG
1	A	343	THR
1	A	351	GLU
1	A	352	ARG
1	A	354	GLN
1	A	360	ASN
1	A	369	VAL
1	A	382	LEU
1	A	397	LEU
1	A	417	ASP
1	B	18	ARG
1	B	20	VAL
1	B	25	PRO
1	B	35	SER
1	B	37	CYS
1	B	40	LEU
1	B	76	LEU
1	B	80	ILE
1	B	86	LEU
1	B	107	LEU
1	B	118	LYS
1	B	119	LEU
1	B	155	LEU
1	B	165	ARG
1	B	171	ILE
1	B	180	MSE
1	B	209	ILE
1	B	223	LEU
1	B	290	LEU
1	B	293	VAL
1	B	305	SER
1	B	317	ASN
1	B	331	GLU
1	B	336	LYS
1	B	346	ASN
1	B	352	ARG
1	B	369	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	382	LEU
1	B	384	LYS
1	B	397	LEU
1	B	416	ILE
1	B	417	ASP
1	C	20	VAL
1	C	25	PRO
1	C	33	THR
1	C	40	LEU
1	C	44	ASP
1	C	76	LEU
1	C	86	LEU
1	C	107	LEU
1	C	119	LEU
1	C	140	ILE
1	C	155	LEU
1	C	162	GLN
1	C	223	LEU
1	C	274	ARG
1	C	281	THR
1	C	290	LEU
1	C	347	SER
1	C	351	GLU
1	C	369	VAL
1	C	397	LEU
1	C	399	ARG
1	D	33	THR
1	D	37	CYS
1	D	40	LEU
1	D	76	LEU
1	D	86	LEU
1	D	105	SER
1	D	107	LEU
1	D	119	LEU
1	D	136	GLU
1	D	155	LEU
1	D	161	THR
1	D	200	PRO
1	D	223	LEU
1	D	290	LEU
1	D	305	SER
1	D	343	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	360	ASN
1	D	363	CYS
1	D	369	VAL
1	D	382	LEU
1	D	397	LEU
1	D	401	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	30	GLN
1	A	55	HIS
1	A	150	HIS
1	A	160	ASN
1	A	162	GLN
1	A	187	GLN
1	A	199	HIS
1	A	359	ASN
1	B	29	HIS
1	B	55	HIS
1	B	187	GLN
1	B	199	HIS
1	B	218	HIS
1	B	317	ASN
1	C	29	HIS
1	C	162	GLN
1	C	187	GLN
1	C	359	ASN
1	D	29	HIS
1	D	55	HIS
1	D	81	GLN
1	D	162	GLN
1	D	199	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	398/421 (94%)	-0.38	6 (1%) 72 74	26, 41, 70, 91	0
1	B	394/421 (93%)	-0.50	2 (0%) 87 88	22, 38, 66, 97	0
1	C	402/421 (95%)	-0.46	6 (1%) 72 74	23, 39, 69, 99	0
1	D	392/421 (93%)	-0.26	4 (1%) 79 80	31, 46, 73, 89	0
All	All	1586/1684 (94%)	-0.40	18 (1%) 78 79	22, 42, 71, 99	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	PHE	3.7
1	A	348	PHE	3.6
1	C	347	SER	3.5
1	A	417	ASP	3.4
1	B	275	ALA	3.2
1	C	152	SER	3.1
1	A	351	GLU	3.0
1	D	275	ALA	3.0
1	C	351	GLU	2.9
1	A	275	ALA	2.7
1	D	417	ASP	2.6
1	C	399	ARG	2.6
1	D	151	SER	2.5
1	A	173	GLY	2.2
1	B	418	TYR	2.2
1	A	272	LYS	2.2
1	C	350	ALA	2.1
1	D	272	LYS	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.