



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:17 PM UTC

PDB ID : 2DWQ / pdb_00002dwq
Title : Thermus thermophilus YchF GTP-binding protein
Authors : Kukimoto-Niino, M.; Murayama, K.; Shorouzu, M.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-08-16
Resolution : 2.95 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

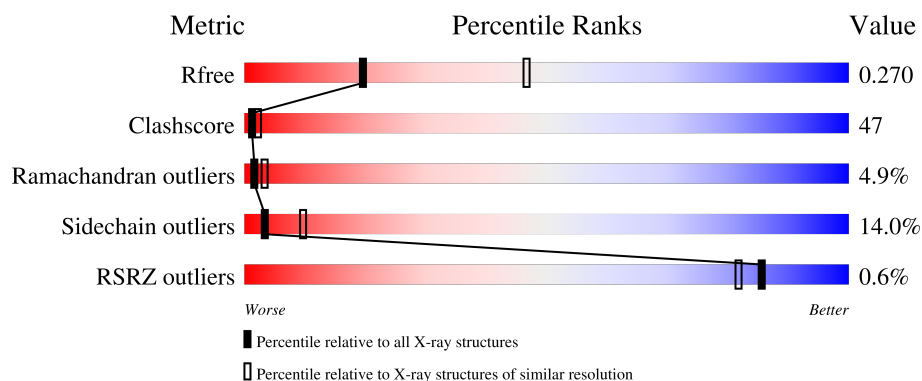
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	368	30% 46% 18% • •
1	B	368	26% 45% 18% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5410 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 GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2748	1739	496	510	3			
1	B	337	Total	C	N	O	S	0	0	0
			2631	1668	475	486	2			

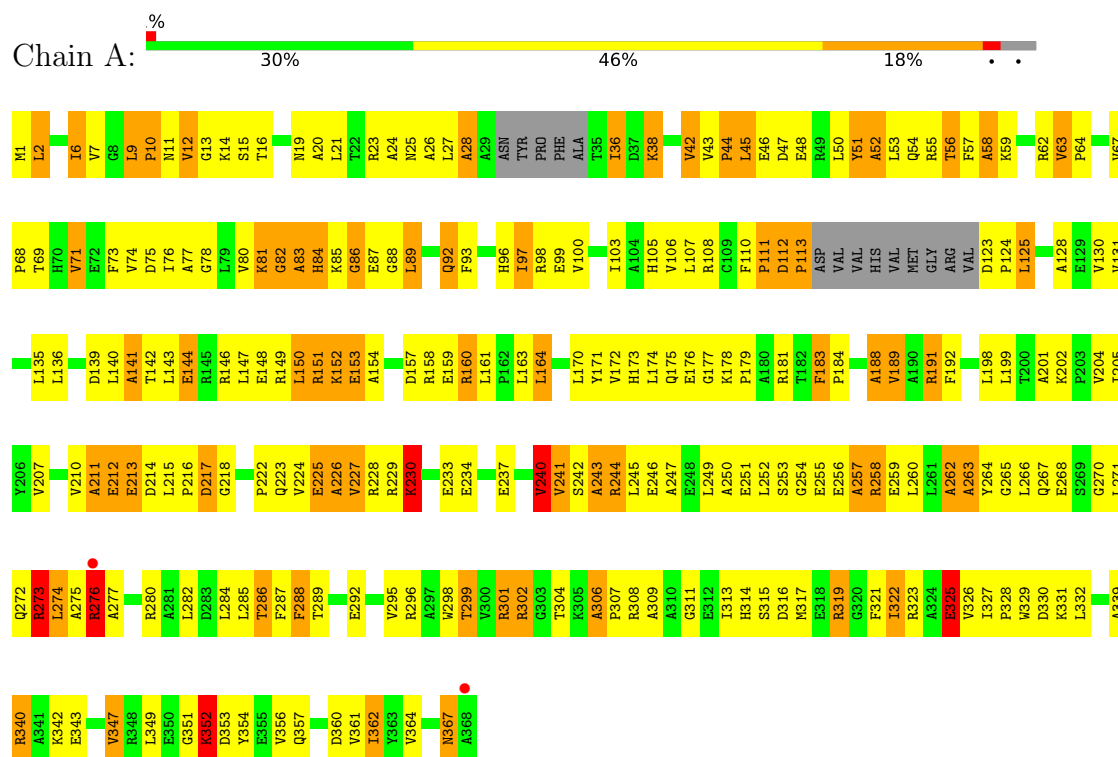
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	9	Total	O	0	0
			9	9		

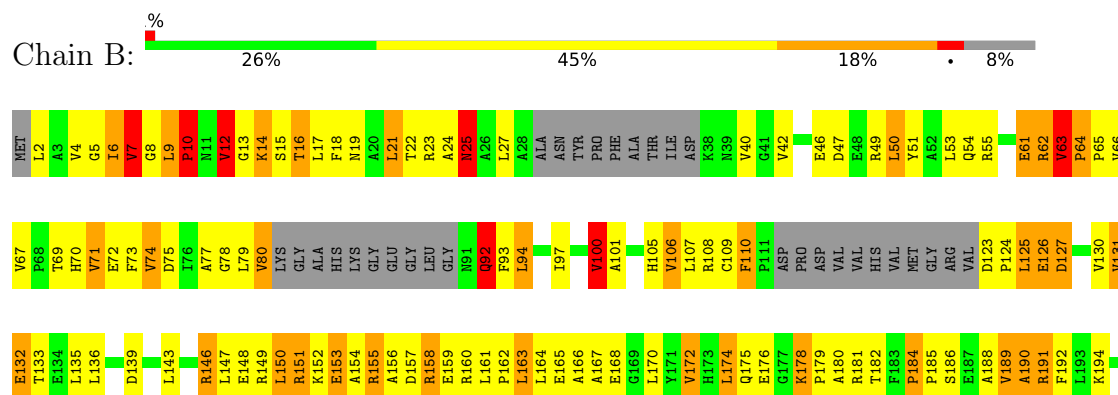
3 Residue-property plots

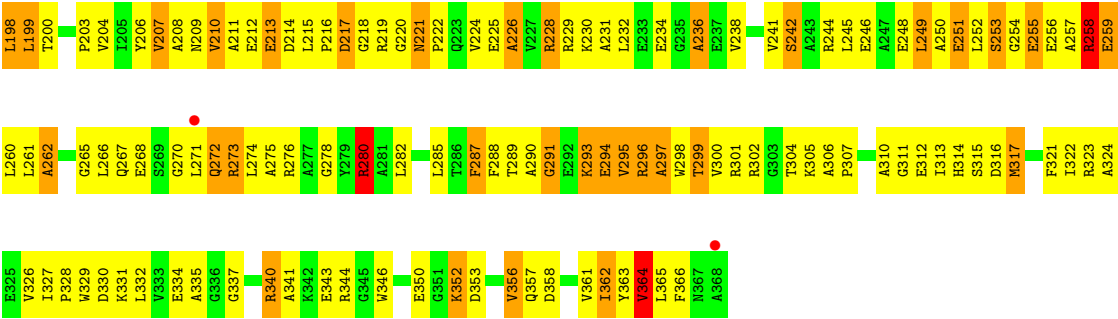
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: GTP-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.94Å 54.36Å 92.58Å 80.11° 76.46° 73.12°	Depositor
Resolution (Å)	37.04 – 2.95 37.04 – 2.95	Depositor EDS
% Data completeness (in resolution range)	94.2 (37.04-2.95) 94.4 (37.04-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.281 0.200 , 0.270	Depositor DCC
R_{free} test set	1872 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5410	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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	1.20	8/2795 (0.3%)	1.58	63/3787 (1.7%)
1	B	0.94	3/2675 (0.1%)	1.46	51/3625 (1.4%)
All	All	1.08	11/5470 (0.2%)	1.52	114/7412 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	VAL	CA-CB	-6.73	1.46	1.54
1	A	103	ILE	CA-CB	6.50	1.62	1.54
1	A	36	ILE	CA-CB	6.39	1.60	1.53
1	A	100	VAL	CA-CB	6.33	1.64	1.55
1	B	71	VAL	CA-CB	6.15	1.62	1.54
1	A	52	ALA	CA-CB	-5.94	1.44	1.53
1	A	58	ALA	CA-CB	-5.52	1.45	1.53
1	B	7	VAL	CA-CB	-5.50	1.47	1.54
1	A	227	VAL	CA-C	-5.20	1.46	1.52
1	B	4	VAL	CA-CB	5.19	1.60	1.54
1	A	43	VAL	CA-C	5.07	1.58	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	VAL	N-CA-C	-17.32	97.57	112.12
1	B	158	ARG	N-CA-C	10.79	122.62	111.07
1	A	84	HIS	N-CA-C	9.78	128.13	107.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ARG	N-CA-C	-9.76	100.50	111.82
1	B	296	ARG	N-CA-C	9.33	124.24	109.50
1	B	184	PRO	CA-C-N	9.32	129.36	119.76
1	B	184	PRO	C-N-CA	9.32	129.36	119.76
1	A	67	VAL	CA-C-N	-8.97	111.38	120.98
1	A	67	VAL	C-N-CA	-8.97	111.38	120.98
1	A	257	ALA	N-CA-C	-8.88	100.77	111.69
1	A	367	ASN	N-CA-C	8.71	124.24	111.96
1	B	50	LEU	N-CA-C	-8.68	100.81	111.40
1	A	362	ILE	N-CA-C	8.45	121.06	108.46
1	A	306	ALA	CA-C-N	-8.10	109.72	119.84
1	A	306	ALA	C-N-CA	-8.10	109.72	119.84
1	A	63	VAL	CA-C-N	-8.05	112.09	120.38
1	A	63	VAL	C-N-CA	-8.05	112.09	120.38
1	A	62	ARG	N-CA-C	-8.04	97.50	110.20
1	A	277	ALA	N-CA-C	-7.90	102.66	111.82
1	B	9	LEU	CA-C-N	7.77	129.55	119.84
1	B	9	LEU	C-N-CA	7.77	129.55	119.84
1	A	89	LEU	N-CA-C	-7.60	103.08	111.36
1	B	178	LYS	CA-C-N	7.53	127.53	119.78
1	B	178	LYS	C-N-CA	7.53	127.53	119.78
1	B	276	ARG	N-CA-C	-7.53	103.05	111.71
1	A	160	ARG	N-CA-C	-7.50	103.26	113.30
1	B	64	PRO	CA-C-N	7.40	127.16	119.76
1	B	64	PRO	C-N-CA	7.40	127.16	119.76
1	A	213	GLU	N-CA-C	-7.37	104.28	113.20
1	A	83	ALA	CA-C-N	-7.37	112.34	122.95
1	A	83	ALA	C-N-CA	-7.37	112.34	122.95
1	A	2	LEU	N-CA-C	-7.34	98.08	109.76
1	A	69	THR	N-CA-C	-7.23	99.76	110.46
1	A	289	THR	N-CA-C	-7.07	98.21	109.59
1	B	210	VAL	N-CA-C	7.06	117.14	108.53
1	A	262	ALA	N-CA-C	-6.96	103.62	111.07
1	A	225	GLU	N-CA-C	-6.94	104.94	113.41
1	B	219	ARG	N-CA-C	-6.91	99.59	109.96
1	A	325	GLU	N-CA-C	-6.86	98.44	109.96
1	A	67	VAL	CB-CA-C	-6.84	103.31	111.18
1	A	286	THR	N-CA-C	6.81	120.61	109.85
1	B	334	GLU	N-CA-C	-6.81	103.98	112.90
1	B	92	GLN	N-CA-C	-6.80	102.25	112.04
1	B	297	ALA	N-CA-C	6.74	119.12	108.67
1	B	361	VAL	N-CA-C	-6.64	98.90	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	VAL	N-CA-C	6.64	115.46	108.95
1	A	28	ALA	N-CA-C	6.58	118.40	108.46
1	B	337	GLY	N-CA-C	6.53	119.78	111.09
1	A	144	GLU	N-CA-C	-6.52	103.29	111.11
1	A	183	PHE	CA-C-N	6.48	127.05	120.38
1	A	183	PHE	C-N-CA	6.48	127.05	120.38
1	A	27	LEU	N-CA-C	-6.38	99.25	109.39
1	B	69	THR	N-CA-C	-6.38	100.77	110.14
1	B	62	ARG	N-CA-C	6.33	120.09	108.58
1	B	228	ARG	N-CA-C	-6.30	104.49	111.36
1	A	52	ALA	N-CA-C	-6.23	103.63	111.11
1	B	364	VAL	N-CA-C	6.21	118.33	108.89
1	A	251	GLU	N-CA-C	6.19	121.06	112.45
1	B	289	THR	N-CA-C	-6.17	98.58	109.06
1	A	211	ALA	N-CA-C	-6.16	100.73	109.96
1	A	86	GLY	N-CA-C	-6.15	98.61	113.18
1	B	106	VAL	CB-CA-C	-6.12	102.14	111.69
1	B	61	GLU	N-CA-C	-6.08	105.62	113.16
1	B	280	ARG	N-CA-C	-6.05	104.68	111.28
1	A	299	THR	N-CA-C	6.04	119.31	109.59
1	A	141	ALA	N-CA-C	-6.02	104.41	110.97
1	A	352	LYS	CA-C-N	-6.02	113.07	123.25
1	A	352	LYS	C-N-CA	-6.02	113.07	123.25
1	A	230	LYS	N-CA-C	-5.97	104.41	111.03
1	B	362	ILE	N-CA-C	5.96	118.28	108.99
1	B	153	GLU	N-CA-C	-5.93	104.81	111.28
1	A	347	VAL	CB-CA-C	-5.83	103.83	111.81
1	B	131	VAL	CB-CA-C	-5.80	103.58	112.05
1	B	226	ALA	N-CA-C	-5.78	104.89	111.07
1	B	190	ALA	N-CA-C	-5.75	107.26	114.56
1	B	133	THR	N-CA-C	-5.70	104.45	111.40
1	B	178	LYS	N-CA-C	-5.67	102.48	110.31
1	A	153	GLU	N-CA-C	-5.59	104.57	111.33
1	A	10	PRO	N-CA-C	5.58	120.26	111.38
1	A	178	LYS	CA-C-N	5.56	126.03	120.14
1	A	178	LYS	C-N-CA	5.56	126.03	120.14
1	A	322	ILE	N-CA-C	-5.55	106.29	111.45
1	B	100	VAL	CB-CA-C	-5.55	102.19	111.29
1	B	172	VAL	CB-CA-C	-5.53	104.79	112.04
1	A	273	ARG	CA-C-N	5.44	127.57	120.28
1	A	273	ARG	C-N-CA	5.44	127.57	120.28
1	A	258	ARG	N-CA-C	-5.44	104.38	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ALA	N-CA-C	5.42	118.68	111.75
1	A	92	GLN	N-CA-C	-5.38	105.42	111.28
1	B	291	GLY	N-CA-C	-5.34	102.35	111.27
1	B	126	GLU	N-CA-C	5.33	116.95	111.03
1	A	243	ALA	N-CA-C	-5.29	104.93	111.33
1	A	240	VAL	CB-CA-C	-5.28	103.98	111.21
1	A	276	ARG	N-CA-C	-5.28	106.97	113.41
1	B	12	VAL	CB-CA-C	-5.28	105.74	110.91
1	A	191	ARG	N-CA-C	-5.25	105.23	111.69
1	B	198	LEU	N-CA-C	-5.23	101.18	109.59
1	A	237	GLU	N-CA-C	-5.22	102.80	110.52
1	A	164	LEU	N-CA-C	-5.19	105.31	110.97
1	A	28	ALA	CA-C-N	5.17	131.01	121.70
1	A	28	ALA	C-N-CA	5.17	131.01	121.70
1	A	205	ILE	CB-CA-C	-5.14	104.85	111.53
1	B	272	GLN	N-CA-C	-5.12	105.70	111.28
1	A	226	ALA	O-C-N	5.12	127.34	122.07
1	B	25	ASN	N-CA-C	-5.10	105.90	111.82
1	B	72	GLU	N-CA-C	5.09	117.06	108.96
1	B	236	ALA	N-CA-C	5.08	117.72	109.24
1	A	131	VAL	CA-C-N	-5.04	113.77	120.63
1	A	131	VAL	C-N-CA	-5.04	113.77	120.63
1	A	316	ASP	N-CA-C	-5.04	105.91	111.71
1	B	299	THR	N-CA-C	5.04	117.97	109.95
1	B	125	LEU	N-CA-C	-5.02	106.99	113.01
1	B	27	LEU	N-CA-C	-5.01	104.42	110.44
1	B	364	VAL	CB-CA-C	-5.01	102.88	110.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2748	0	2784	233	0
1	B	2631	0	2666	290	0
2	A	22	0	0	6	0
2	B	9	0	0	2	0
All	All	5410	0	5450	510	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 47.

All (510) 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:23:ARG:HE	1:B:251:GLU:HG2	0.95	1.08
1:A:16:THR:HB	1:A:243:ALA:HB1	1.37	1.05
1:A:302:ARG:HH11	1:A:302:ARG:HB2	1.18	1.04
1:A:244:ARG:HG3	1:A:244:ARG:HH11	1.24	1.02
1:B:258:ARG:HE	1:B:258:ARG:HA	1.24	1.02
1:A:302:ARG:HB2	1:A:302:ARG:NH1	1.75	1.01
1:B:23:ARG:NE	1:B:251:GLU:HG2	1.76	0.99
1:A:340:ARG:HD3	1:B:267:GLN:CB	1.91	0.99
1:B:340:ARG:HG2	1:B:340:ARG:HH11	1.30	0.95
1:B:293:LYS:HD2	1:B:294:GLU:H	1.32	0.94
1:B:14:LYS:HZ3	1:B:77:ALA:HB2	1.33	0.92
1:A:85:LYS:HB3	1:A:92:GLN:HE22	1.34	0.90
1:A:302:ARG:HH11	1:A:302:ARG:CB	1.84	0.90
1:B:147:LEU:O	1:B:151:ARG:HB2	1.70	0.90
1:A:98:ARG:HG3	1:A:199:LEU:HD21	1.52	0.89
1:A:260:LEU:HD11	1:A:264:TYR:HE1	1.36	0.88
1:A:340:ARG:HD3	1:B:267:GLN:HB3	1.55	0.88
1:A:63:VAL:HG22	1:A:64:PRO:HD2	1.54	0.88
1:A:340:ARG:HD3	1:B:267:GLN:HB2	1.56	0.86
1:B:23:ARG:HE	1:B:251:GLU:CG	1.86	0.86
1:A:244:ARG:HG3	1:A:244:ARG:NH1	1.88	0.86
1:A:340:ARG:HG3	2:A:371:HOH:O	1.77	0.85
1:B:5:GLY:HA3	1:B:100:VAL:HG11	1.61	0.82
1:A:260:LEU:O	1:A:263:ALA:HB3	1.80	0.81
1:A:319:ARG:HG2	1:A:319:ARG:HH11	1.44	0.81
1:B:61:GLU:HB2	1:B:62:ARG:HH11	1.45	0.81
1:A:322:ILE:O	1:A:323:ARG:HG2	1.81	0.80
1:A:245:LEU:HG	1:A:249:LEU:HD11	1.66	0.78
1:B:158:ARG:HD2	1:B:159:GLU:N	1.98	0.77
1:B:40:VAL:HG22	1:B:74:VAL:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ARG:HD3	2:B:376:HOH:O	1.83	0.77
1:A:171:TYR:CE2	1:A:175:GLN:NE2	2.52	0.76
1:A:54:GLN:HG2	1:A:63:VAL:CG2	2.15	0.76
1:A:215:LEU:CD1	1:A:245:LEU:HD23	2.16	0.76
1:A:260:LEU:O	1:A:260:LEU:HD12	1.85	0.75
1:A:367:ASN:HD22	1:A:367:ASN:C	1.94	0.75
1:A:260:LEU:HD11	1:A:264:TYR:CE1	2.21	0.75
1:A:88:GLY:O	1:A:92:GLN:HG3	1.86	0.75
1:B:14:LYS:HA	1:B:106:VAL:HG21	1.68	0.74
1:A:98:ARG:HG3	1:A:199:LEU:CD2	2.16	0.74
1:B:291:GLY:HA3	1:B:293:LYS:HE3	1.69	0.74
1:B:25:ASN:HD22	1:B:25:ASN:C	1.93	0.74
1:B:188:ALA:C	1:B:190:ALA:H	1.96	0.74
1:B:340:ARG:HG2	1:B:340:ARG:NH1	2.02	0.74
1:B:285:LEU:HD12	1:B:285:LEU:O	1.86	0.74
1:B:78:GLY:O	1:B:80:VAL:N	2.21	0.73
1:A:258:ARG:HE	1:A:258:ARG:HA	1.53	0.73
1:B:244:ARG:HH11	1:B:244:ARG:HB3	1.54	0.72
1:B:322:ILE:O	1:B:323:ARG:HD3	1.90	0.72
1:B:246:GLU:OE2	1:B:271:LEU:HD12	1.90	0.72
1:A:25:ASN:O	1:A:28:ALA:HB3	1.89	0.72
1:A:314:HIS:ND1	1:A:315:SER:N	2.38	0.71
1:B:322:ILE:HD12	1:B:366:PHE:HA	1.70	0.71
1:B:244:ARG:HB2	1:B:244:ARG:NH1	2.05	0.70
1:A:12:VAL:HG12	1:A:108:ARG:HB3	1.72	0.70
1:B:244:ARG:NH1	1:B:244:ARG:CB	2.54	0.70
1:B:322:ILE:HG22	1:B:323:ARG:HG2	1.72	0.70
1:A:170:LEU:O	1:A:174:LEU:HD12	1.90	0.70
1:A:59:LYS:HD3	1:A:292:GLU:OE1	1.92	0.70
1:A:215:LEU:HD11	1:A:245:LEU:HD23	1.74	0.70
1:B:206:TYR:HB2	1:B:238:VAL:HG22	1.74	0.70
1:A:224:VAL:HG12	1:A:224:VAL:O	1.90	0.70
1:A:240:VAL:O	1:A:241:VAL:HG13	1.91	0.70
1:B:139:ASP:OD2	1:B:198:LEU:HB3	1.91	0.69
1:A:326:VAL:HG22	1:A:362:ILE:HG12	1.74	0.69
1:A:267:GLN:HG3	1:B:340:ARG:CZ	2.23	0.69
1:B:244:ARG:HH11	1:B:244:ARG:CB	2.05	0.69
1:B:152:LYS:O	1:B:152:LYS:HD3	1.94	0.68
1:B:158:ARG:O	1:B:161:LEU:HD13	1.93	0.68
1:A:63:VAL:HG22	1:A:64:PRO:CD	2.22	0.68
1:B:189:VAL:HG12	1:B:189:VAL:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLY:O	1:B:282:LEU:HG	1.94	0.68
1:B:78:GLY:C	1:B:80:VAL:H	2.01	0.67
1:B:285:LEU:HD21	1:B:302:ARG:HA	1.76	0.67
1:B:92:GLN:HA	1:B:92:GLN:OE1	1.92	0.67
1:A:80:VAL:HG21	1:A:93:PHE:CD1	2.30	0.67
1:B:5:GLY:CA	1:B:100:VAL:HG11	2.25	0.67
1:A:188:ALA:O	1:A:189:VAL:C	2.38	0.67
1:B:8:GLY:O	1:B:10:PRO:HD3	1.95	0.66
1:B:49:ARG:O	1:B:53:LEU:HB2	1.96	0.66
1:B:212:GLU:O	1:B:215:LEU:HB2	1.95	0.65
1:B:61:GLU:HB2	1:B:62:ARG:NH1	2.10	0.65
1:B:285:LEU:CD2	1:B:302:ARG:HA	2.27	0.65
1:B:226:ALA:O	1:B:229:ARG:HB3	1.97	0.65
1:A:259:GLU:O	1:A:262:ALA:HB3	1.96	0.65
1:A:15:SER:O	1:A:19:ASN:HB2	1.98	0.64
1:A:246:GLU:OE1	1:A:270:GLY:N	2.30	0.64
1:B:74:VAL:HG12	1:B:74:VAL:O	1.97	0.64
1:A:2:LEU:HB3	1:A:282:LEU:HD13	1.80	0.64
1:B:127:ASP:O	1:B:131:VAL:HG23	1.98	0.64
1:A:149:ARG:O	1:A:152:LYS:HG3	1.97	0.64
1:B:143:LEU:O	1:B:147:LEU:HB2	1.97	0.64
1:A:276:ARG:HB2	1:A:280:ARG:HH12	1.62	0.64
1:B:216:PRO:HG2	1:B:217:ASP:OD2	1.97	0.63
1:B:16:THR:O	1:B:19:ASN:HB3	1.99	0.63
1:B:335:ALA:HB2	1:B:346:TRP:CZ3	2.32	0.63
1:A:152:LYS:C	1:A:152:LYS:HD2	2.23	0.63
1:A:23:ARG:O	1:A:26:ALA:HB3	1.99	0.63
1:B:229:ARG:HG2	1:B:229:ARG:HH11	1.64	0.63
1:B:293:LYS:HD2	1:B:294:GLU:N	2.10	0.63
1:A:36:ILE:HD13	1:A:38:LYS:HE2	1.78	0.63
1:A:124:PRO:HA	2:A:382:HOH:O	1.97	0.63
1:B:256:GLU:O	1:B:257:ALA:C	2.40	0.63
1:B:253:SER:O	1:B:256:GLU:HB3	1.99	0.63
1:B:135:LEU:HD23	1:B:199:LEU:HD12	1.81	0.63
1:A:240:VAL:O	1:A:241:VAL:CG1	2.47	0.62
1:B:67:VAL:HG12	1:B:296:ARG:HG3	1.82	0.62
1:B:254:GLY:C	1:B:256:GLU:H	2.06	0.62
1:B:186:SER:HB3	1:B:189:VAL:CG2	2.29	0.62
1:B:340:ARG:O	1:B:343:GLU:HB2	2.00	0.62
1:B:181:ARG:NH2	1:B:204:VAL:HG21	2.15	0.61
1:B:158:ARG:NH1	1:B:159:GLU:HB2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:O	1:B:165:GLU:HG3	2.00	0.61
1:B:50:LEU:HD23	1:B:288:PHE:CE2	2.35	0.61
1:B:317:MET:HG3	1:B:366:PHE:CE2	2.35	0.61
1:A:54:GLN:HG2	1:A:63:VAL:HG22	1.82	0.61
1:A:54:GLN:HG2	1:A:63:VAL:HG21	1.81	0.61
1:B:152:LYS:HD3	1:B:152:LYS:C	2.24	0.61
1:A:150:LEU:HD23	1:A:153:GLU:OE2	1.99	0.61
1:B:15:SER:O	1:B:16:THR:C	2.44	0.61
1:B:154:ALA:HA	1:B:160:ARG:HB2	1.82	0.61
1:B:228:ARG:O	1:B:232:LEU:HD23	2.01	0.61
1:A:47:ASP:O	1:A:50:LEU:HB2	2.01	0.61
1:A:330:ASP:OD2	1:A:330:ASP:N	2.33	0.61
1:A:340:ARG:CD	1:B:267:GLN:HB3	2.29	0.61
1:A:256:GLU:HA	1:A:259:GLU:HG2	1.83	0.60
1:B:9:LEU:HG	1:B:127:ASP:HB3	1.83	0.60
1:B:258:ARG:HA	1:B:258:ARG:NE	2.08	0.60
1:A:367:ASN:C	1:A:367:ASN:ND2	2.60	0.60
1:B:222:PRO:HA	1:B:225:GLU:HG3	1.83	0.60
1:A:36:ILE:HG12	1:A:38:LYS:HG2	1.84	0.60
1:A:262:ALA:O	1:A:265:GLY:N	2.32	0.60
1:B:77:ALA:O	1:B:80:VAL:HG23	2.01	0.60
1:B:313:ILE:HG21	1:B:317:MET:HE1	1.82	0.60
1:A:151:ARG:HA	1:A:164:LEU:HD11	1.84	0.60
1:B:314:HIS:CE1	1:B:316:ASP:OD1	2.55	0.60
1:B:213:GLU:H	1:B:213:GLU:CD	2.09	0.59
1:A:259:GLU:O	1:A:263:ALA:N	2.28	0.59
1:A:157:ASP:OD2	1:A:157:ASP:C	2.45	0.59
1:B:335:ALA:HB2	1:B:346:TRP:CE3	2.38	0.59
1:B:186:SER:HB3	1:B:189:VAL:HG23	1.84	0.59
1:B:301:ARG:O	1:B:302:ARG:C	2.46	0.59
1:A:255:GLU:O	1:A:258:ARG:HB3	2.03	0.59
1:B:231:ALA:HB1	1:B:236:ALA:O	2.03	0.59
1:B:155:ARG:C	1:B:157:ASP:H	2.11	0.59
1:A:319:ARG:HD2	1:A:319:ARG:C	2.28	0.58
1:B:73:PHE:CZ	1:B:274:LEU:HG	2.37	0.58
1:B:317:MET:HG3	1:B:366:PHE:CD2	2.39	0.58
1:A:172:VAL:O	1:A:176:GLU:HG3	2.01	0.58
1:B:188:ALA:C	1:B:190:ALA:N	2.61	0.58
1:B:214:ASP:O	1:B:218:GLY:HA2	2.04	0.58
1:A:7:VAL:HG12	1:A:76:ILE:HB	1.86	0.58
1:A:87:GLU:H	1:A:87:GLU:CD	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ARG:HH21	1:B:150:LEU:HG	1.68	0.58
1:B:24:ALA:HB2	1:B:250:ALA:O	2.04	0.58
1:A:298:TRP:CH2	1:A:313:ILE:HA	2.39	0.57
1:B:154:ALA:HB1	1:B:164:LEU:HD22	1.85	0.57
1:A:7:VAL:HG11	1:A:97:ILE:HD11	1.85	0.57
1:B:135:LEU:CD2	1:B:199:LEU:HD12	2.34	0.57
1:B:245:LEU:O	1:B:249:LEU:HG	2.05	0.57
1:A:108:ARG:O	1:A:124:PRO:HB3	2.03	0.57
1:B:46:GLU:HB2	1:B:272:GLN:OE1	2.03	0.57
1:B:132:GLU:O	1:B:136:LEU:HG	2.03	0.57
1:A:77:ALA:O	1:A:78:GLY:C	2.48	0.57
1:A:276:ARG:HH12	1:B:344:ARG:CZ	2.17	0.57
1:B:106:VAL:HA	1:B:207:VAL:HB	1.87	0.57
1:B:273:ARG:HG2	1:B:273:ARG:HH11	1.70	0.57
1:A:42:VAL:O	1:A:44:PRO:HD3	2.05	0.57
1:A:58:ALA:HB2	1:A:63:VAL:HG23	1.86	0.56
1:A:244:ARG:O	1:A:247:ALA:HB3	2.05	0.56
1:A:357:GLN:O	1:A:360:ASP:HB2	2.05	0.56
1:A:85:LYS:HB3	1:A:92:GLN:NE2	2.14	0.56
1:A:150:LEU:CD1	1:A:164:LEU:HD12	2.35	0.56
1:B:62:ARG:N	1:B:62:ARG:CD	2.68	0.56
1:B:154:ALA:CB	1:B:164:LEU:HD22	2.35	0.56
1:B:285:LEU:HD12	1:B:285:LEU:C	2.30	0.56
1:A:256:GLU:O	1:A:259:GLU:HG3	2.05	0.56
1:B:13:GLY:O	1:B:14:LYS:C	2.49	0.56
1:A:319:ARG:HG2	1:A:319:ARG:NH1	2.16	0.56
1:A:97:ILE:O	1:A:202:LYS:HE3	2.06	0.56
1:A:214:ASP:O	1:A:215:LEU:C	2.48	0.56
1:B:54:GLN:NE2	1:B:66:VAL:HG13	2.21	0.56
1:B:71:VAL:CG2	1:B:275:ALA:HB1	2.35	0.56
1:A:215:LEU:HD13	1:A:266:LEU:HD11	1.88	0.56
1:A:351:GLY:O	1:A:353:ASP:N	2.39	0.56
1:B:305:LYS:HD3	1:B:353:ASP:HA	1.86	0.56
1:A:10:PRO:HA	2:A:389:HOH:O	2.05	0.56
1:A:288:PHE:HB3	1:A:296:ARG:O	2.05	0.55
1:B:364:VAL:HG12	1:B:365:LEU:N	2.21	0.55
1:A:252:LEU:HD11	1:A:260:LEU:HD23	1.88	0.55
1:A:254:GLY:O	1:A:258:ARG:HB2	2.06	0.55
1:B:7:VAL:HG23	1:B:8:GLY:N	2.21	0.55
1:B:260:LEU:O	1:B:261:LEU:C	2.50	0.55
1:B:135:LEU:HD22	1:B:199:LEU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:GLU:OE1	1:B:200:THR:HG22	2.07	0.55
1:A:181:ARG:HD2	1:A:234:GLU:O	2.06	0.55
1:B:256:GLU:C	1:B:258:ARG:N	2.60	0.54
1:A:260:LEU:HD12	1:A:263:ALA:HB3	1.89	0.54
1:B:147:LEU:O	1:B:151:ARG:CB	2.50	0.54
1:B:225:GLU:O	1:B:229:ARG:HB2	2.07	0.54
1:B:321:PHE:HE1	1:B:324:ALA:HB2	1.72	0.54
1:B:188:ALA:O	1:B:190:ALA:N	2.41	0.54
1:B:290:ALA:CB	1:B:295:VAL:HG23	2.38	0.54
1:B:328:PRO:HG2	1:B:331:LYS:HG2	1.89	0.54
1:B:109:CYS:SG	1:B:224:VAL:HG22	2.48	0.54
1:A:276:ARG:HH12	1:B:344:ARG:NH2	2.05	0.54
1:A:282:LEU:N	1:A:282:LEU:HD23	2.22	0.54
1:B:14:LYS:HE2	1:B:75:ASP:OD1	2.07	0.54
1:B:65:PRO:CD	1:B:293:LYS:O	2.56	0.54
1:A:328:PRO:HB2	1:A:330:ASP:OD2	2.09	0.53
1:B:6:ILE:HD11	1:B:73:PHE:HD2	1.73	0.53
1:B:244:ARG:HB2	1:B:244:ARG:CZ	2.38	0.53
1:B:254:GLY:C	1:B:256:GLU:N	2.67	0.53
1:A:210:VAL:HG11	1:A:224:VAL:HG21	1.89	0.53
1:A:240:VAL:C	1:A:241:VAL:HG13	2.32	0.53
1:A:189:VAL:O	1:A:192:PHE:N	2.41	0.53
1:B:92:GLN:O	1:B:93:PHE:C	2.51	0.53
1:B:230:LYS:HE2	1:B:234:GLU:HG3	1.91	0.53
1:B:151:ARG:HA	1:B:164:LEU:HD13	1.90	0.53
1:A:223:GLN:C	1:A:225:GLU:H	2.16	0.53
1:A:280:ARG:HG3	1:A:280:ARG:HH11	1.73	0.53
1:A:150:LEU:HD13	1:A:164:LEU:CD1	2.39	0.53
1:A:225:GLU:O	1:A:229:ARG:HG3	2.08	0.53
1:B:101:ALA:O	1:B:203:PRO:HD2	2.09	0.53
1:B:13:GLY:O	1:B:15:SER:N	2.42	0.53
1:B:186:SER:C	1:B:188:ALA:H	2.17	0.52
1:B:73:PHE:CE2	1:B:274:LEU:HD21	2.44	0.52
1:A:212:GLU:OE1	1:A:244:ARG:HG2	2.09	0.52
1:B:127:ASP:OD2	1:B:127:ASP:N	2.42	0.52
1:A:309:ALA:HB2	1:A:356:VAL:HG21	1.91	0.52
1:B:65:PRO:HD2	1:B:293:LYS:O	2.08	0.52
1:A:170:LEU:O	1:A:173:HIS:HB3	2.10	0.52
1:A:214:ASP:C	1:A:215:LEU:O	2.50	0.52
1:A:267:GLN:HG2	1:B:340:ARG:CG	2.39	0.52
1:B:252:LEU:HD12	1:B:260:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HH11	1:B:340:ARG:CG	2.12	0.52
1:A:256:GLU:O	1:A:259:GLU:CG	2.57	0.52
1:A:276:ARG:O	1:A:280:ARG:NH1	2.43	0.52
1:B:221:ASN:CG	1:B:224:VAL:HG23	2.34	0.52
1:B:71:VAL:HG21	1:B:275:ALA:HB1	1.92	0.51
1:B:150:LEU:HD23	1:B:153:GLU:OE2	2.10	0.51
1:A:211:ALA:O	1:A:214:ASP:HB2	2.10	0.51
1:B:161:LEU:HB2	1:B:162:PRO:HD3	1.92	0.51
1:B:14:LYS:HZ3	1:B:77:ALA:CB	2.14	0.51
1:B:296:ARG:HD3	1:B:298:TRP:CZ2	2.46	0.51
1:A:125:LEU:O	1:A:128:ALA:HB3	2.10	0.51
1:B:189:VAL:O	1:B:189:VAL:CG1	2.58	0.51
1:A:304:THR:HG23	1:A:308:ARG:HB3	1.91	0.51
1:B:70:HIS:ND1	1:B:70:HIS:N	2.59	0.51
1:B:148:GLU:O	1:B:149:ARG:C	2.52	0.51
1:B:256:GLU:O	1:B:259:GLU:N	2.43	0.51
1:B:329:TRP:CG	1:B:330:ASP:N	2.78	0.51
1:A:259:GLU:O	1:A:262:ALA:N	2.44	0.51
1:A:10:PRO:CA	2:A:389:HOH:O	2.58	0.50
1:B:17:LEU:C	1:B:19:ASN:H	2.19	0.50
1:A:13:GLY:O	1:A:14:LYS:C	2.53	0.50
1:A:85:LYS:CB	1:A:92:GLN:HE22	2.16	0.50
1:B:262:ALA:O	1:B:265:GLY:N	2.43	0.50
1:A:319:ARG:NH1	1:A:319:ARG:CG	2.74	0.50
1:B:242:SER:O	1:B:246:GLU:HG2	2.11	0.50
1:B:311:GLY:C	1:B:313:ILE:N	2.69	0.50
1:B:62:ARG:N	1:B:62:ARG:HD3	2.26	0.50
1:B:307:PRO:HG2	1:B:352:LYS:HB2	1.93	0.50
1:A:96:HIS:C	1:A:98:ARG:N	2.69	0.50
1:A:217:ASP:OD1	1:A:273:ARG:NH2	2.45	0.50
1:A:301:ARG:O	1:A:302:ARG:C	2.55	0.50
1:B:17:LEU:C	1:B:19:ASN:N	2.70	0.50
1:A:85:LYS:HG2	1:A:87:GLU:O	2.12	0.50
1:A:272:GLN:O	1:A:273:ARG:C	2.52	0.50
1:A:259:GLU:HG3	1:A:260:LEU:H	1.76	0.50
1:B:18:PHE:O	1:B:18:PHE:CD2	2.65	0.50
1:B:2:LEU:HD11	1:B:301:ARG:HH21	1.75	0.50
1:B:110:PHE:CD2	1:B:110:PHE:O	2.65	0.50
1:B:159:GLU:O	1:B:162:PRO:HD2	2.11	0.50
1:B:249:LEU:C	1:B:251:GLU:N	2.68	0.50
1:B:261:LEU:HB3	1:B:266:LEU:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ARG:HG2	1:B:273:ARG:NH1	2.25	0.50
1:B:210:VAL:HG23	1:B:211:ALA:O	2.12	0.49
1:B:249:LEU:O	1:B:251:GLU:N	2.45	0.49
1:A:223:GLN:C	1:A:225:GLU:N	2.70	0.49
1:A:150:LEU:HD12	1:A:164:LEU:HD12	1.93	0.49
1:A:249:LEU:O	1:A:250:ALA:C	2.55	0.49
1:B:256:GLU:HG3	1:B:259:GLU:HG2	1.95	0.49
1:B:310:ALA:HB1	1:B:317:MET:HB3	1.92	0.49
1:A:322:ILE:O	1:A:323:ARG:CG	2.58	0.49
1:B:255:GLU:HA	1:B:255:GLU:OE1	2.13	0.49
1:B:299:THR:O	1:B:300:VAL:HG13	2.13	0.49
1:A:244:ARG:HH11	1:A:244:ARG:CG	2.07	0.49
1:A:9:LEU:O	1:A:12:VAL:HG22	2.12	0.48
1:A:123:ASP:OD2	1:A:123:ASP:C	2.55	0.48
1:A:150:LEU:CD2	1:A:153:GLU:OE2	2.60	0.48
1:A:160:ARG:NH1	1:A:163:LEU:HD22	2.28	0.48
1:A:306:ALA:N	1:A:354:TYR:O	2.39	0.48
1:B:22:THR:O	1:B:23:ARG:C	2.56	0.48
1:B:221:ASN:OD1	1:B:224:VAL:HG23	2.13	0.48
1:A:183:PHE:CD1	1:A:184:PRO:HD2	2.48	0.48
1:B:322:ILE:HD12	1:B:365:LEU:O	2.13	0.48
1:A:6:ILE:HD11	1:A:73:PHE:CD2	2.48	0.48
1:A:144:GLU:HG3	1:A:171:TYR:CE1	2.48	0.48
1:B:78:GLY:C	1:B:80:VAL:N	2.66	0.48
1:A:216:PRO:HB3	1:A:266:LEU:HD22	1.95	0.48
1:B:307:PRO:O	1:B:310:ALA:HB3	2.14	0.48
1:A:106:VAL:C	1:A:107:LEU:HD23	2.38	0.48
1:B:12:VAL:HG12	1:B:108:ARG:CB	2.44	0.48
1:B:25:ASN:C	1:B:25:ASN:ND2	2.65	0.48
1:B:50:LEU:CD2	1:B:288:PHE:CE2	2.96	0.48
1:B:167:ALA:O	1:B:168:GLU:C	2.56	0.48
1:B:254:GLY:O	1:B:256:GLU:N	2.47	0.48
1:A:267:GLN:HG2	1:B:340:ARG:HG3	1.95	0.48
1:B:184:PRO:HA	1:B:185:PRO:HD3	1.66	0.48
1:B:322:ILE:HD12	1:B:366:PHE:CA	2.40	0.48
1:B:65:PRO:HG2	1:B:294:GLU:HA	1.94	0.48
1:B:166:ALA:O	1:B:170:LEU:N	2.42	0.48
1:A:224:VAL:O	1:A:224:VAL:CG1	2.62	0.47
1:A:230:LYS:HE2	1:A:230:LYS:HA	1.95	0.47
1:B:317:MET:O	1:B:321:PHE:HB2	2.13	0.47
1:A:259:GLU:HG3	1:A:260:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD22	1:A:199:LEU:HD13	1.96	0.47
1:A:217:ASP:O	1:A:218:GLY:C	2.56	0.47
1:A:230:LYS:O	1:A:233:GLU:N	2.43	0.47
1:B:172:VAL:O	1:B:176:GLU:HG3	2.14	0.47
1:A:36:ILE:HG23	1:A:36:ILE:O	2.15	0.47
1:A:143:LEU:O	1:A:144:GLU:C	2.57	0.47
1:A:302:ARG:NH1	1:A:302:ARG:CB	2.56	0.47
1:B:220:GLY:O	1:B:222:PRO:HD3	2.14	0.47
1:A:96:HIS:O	1:A:98:ARG:N	2.48	0.47
1:A:150:LEU:HD13	1:A:164:LEU:HD13	1.96	0.47
1:B:124:PRO:C	1:B:126:GLU:H	2.22	0.47
1:B:174:LEU:HD11	1:B:180:ALA:HB2	1.97	0.47
1:B:261:LEU:HB3	1:B:266:LEU:HB2	1.97	0.47
1:A:20:ALA:O	1:A:21:LEU:C	2.58	0.47
1:A:106:VAL:O	1:A:107:LEU:HD23	2.14	0.47
1:A:227:VAL:HG12	1:A:228:ARG:N	2.30	0.47
1:B:229:ARG:HG2	1:B:229:ARG:NH1	2.29	0.47
1:B:364:VAL:HG12	1:B:365:LEU:H	1.78	0.47
1:A:110:PHE:CG	1:A:110:PHE:O	2.68	0.46
1:A:171:TYR:CD2	1:A:175:GLN:NE2	2.79	0.46
1:B:210:VAL:O	1:B:242:SER:HB2	2.14	0.46
1:B:311:GLY:O	1:B:313:ILE:N	2.48	0.46
1:A:253:SER:O	1:A:257:ALA:N	2.39	0.46
1:A:326:VAL:HA	1:A:361:VAL:O	2.14	0.46
1:B:23:ARG:CZ	1:B:251:GLU:HG2	2.43	0.46
1:A:253:SER:O	1:A:254:GLY:C	2.58	0.46
1:B:124:PRO:C	1:B:126:GLU:N	2.70	0.46
1:B:163:LEU:CD1	1:B:192:PHE:HB2	2.45	0.46
1:B:300:VAL:CG1	1:B:304:THR:HG21	2.46	0.46
1:A:136:LEU:HD11	1:A:177:GLY:O	2.15	0.46
1:A:110:PHE:O	1:A:111:PRO:C	2.58	0.46
1:A:198:LEU:O	1:A:201:ALA:HB3	2.15	0.46
1:A:223:GLN:O	1:A:226:ALA:N	2.49	0.46
1:B:66:VAL:HG23	1:B:66:VAL:O	2.16	0.46
1:B:209:ASN:C	1:B:209:ASN:OD1	2.57	0.46
1:B:6:ILE:HD11	1:B:73:PHE:CD2	2.51	0.46
1:B:50:LEU:CD2	1:B:288:PHE:HE2	2.28	0.46
1:B:107:LEU:HB3	1:B:124:PRO:HB2	1.98	0.46
1:B:241:VAL:HG23	1:B:242:SER:N	2.30	0.46
1:B:332:LEU:O	1:B:332:LEU:HG	2.16	0.46
1:A:96:HIS:O	1:A:99:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:PHE:CE2	1:B:274:LEU:HG	2.50	0.46
1:A:351:GLY:O	1:A:352:LYS:C	2.59	0.45
1:A:80:VAL:HG21	1:A:93:PHE:CE1	2.51	0.45
1:A:339:ALA:O	1:A:343:GLU:HG3	2.16	0.45
1:B:47:ASP:OD1	1:B:49:ARG:NH2	2.49	0.45
1:B:188:ALA:O	1:B:191:ARG:N	2.48	0.45
1:A:254:GLY:O	1:A:258:ARG:N	2.44	0.45
1:B:314:HIS:NE2	1:B:316:ASP:OD1	2.49	0.45
1:A:23:ARG:C	1:A:26:ALA:HB3	2.41	0.45
1:B:50:LEU:HD23	1:B:288:PHE:CD2	2.52	0.45
1:B:252:LEU:O	1:B:253:SER:C	2.59	0.45
1:A:80:VAL:HG11	1:A:93:PHE:CD1	2.51	0.45
1:A:81:LYS:O	1:A:82:GLY:C	2.60	0.45
1:A:267:GLN:HG2	1:B:340:ARG:CD	2.47	0.45
1:B:73:PHE:CE2	1:B:274:LEU:CD2	3.00	0.45
1:B:246:GLU:HB3	1:B:271:LEU:HD11	1.99	0.45
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.76	0.45
1:B:21:LEU:C	1:B:21:LEU:HD12	2.42	0.45
1:B:186:SER:C	1:B:188:ALA:N	2.74	0.45
1:B:259:GLU:O	1:B:262:ALA:HB3	2.17	0.45
1:A:317:MET:CE	1:A:364:VAL:HB	2.46	0.45
1:A:327:ILE:HD11	1:A:331:LYS:HB2	1.98	0.45
1:B:15:SER:O	1:B:17:LEU:N	2.50	0.45
1:A:80:VAL:O	1:A:81:LYS:O	2.35	0.45
1:B:221:ASN:HB3	1:B:224:VAL:HB	1.98	0.45
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.71	0.45
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.85	0.45
1:A:307:PRO:HG3	1:A:321:PHE:CD2	2.52	0.44
1:A:326:VAL:HG22	1:A:362:ILE:CG1	2.46	0.44
1:B:136:LEU:HD23	1:B:174:LEU:HD23	1.99	0.44
1:B:194:LYS:HA	2:B:371:HOH:O	2.17	0.44
1:B:9:LEU:O	1:B:12:VAL:HG22	2.17	0.44
1:B:21:LEU:HD11	1:B:42:VAL:N	2.32	0.44
1:B:71:VAL:HG23	1:B:275:ALA:HB1	2.00	0.44
1:B:280:ARG:HH11	1:B:280:ARG:CG	2.30	0.44
1:A:50:LEU:HD22	1:A:295:VAL:HG12	2.00	0.44
1:A:56:THR:HG22	1:A:57:PHE:CE1	2.53	0.44
1:A:241:VAL:HG12	1:A:270:GLY:CA	2.47	0.44
1:A:2:LEU:HD12	1:A:284:LEU:HD21	1.99	0.44
1:A:96:HIS:O	1:A:97:ILE:C	2.59	0.44
1:B:238:VAL:O	1:B:238:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD11	1:A:329:TRP:HB2	2.00	0.44
1:A:285:LEU:C	1:A:285:LEU:HD12	2.43	0.44
1:B:341:ALA:C	1:B:343:GLU:N	2.74	0.44
1:A:214:ASP:O	1:A:215:LEU:O	2.36	0.44
1:B:158:ARG:CZ	1:B:159:GLU:HB2	2.48	0.44
1:B:306:ALA:HB3	1:B:307:PRO:HD3	1.99	0.44
1:B:221:ASN:HA	1:B:222:PRO:HD2	1.86	0.44
1:A:11:ASN:N	2:A:389:HOH:O	2.26	0.44
1:A:68:PRO:HB2	2:A:387:HOH:O	2.18	0.44
1:B:178:LYS:HA	1:B:179:PRO:HD3	1.86	0.44
1:A:309:ALA:C	1:A:311:GLY:N	2.75	0.43
1:B:250:ALA:C	1:B:251:GLU:HG3	2.42	0.43
1:B:244:ARG:HG3	1:B:245:LEU:N	2.33	0.43
1:B:321:PHE:CE1	1:B:324:ALA:HB2	2.53	0.43
1:B:327:ILE:O	1:B:327:ILE:HG23	2.16	0.43
1:A:7:VAL:O	1:A:105:HIS:HA	2.17	0.43
1:B:12:VAL:HG12	1:B:108:ARG:H	1.83	0.43
1:B:164:LEU:O	1:B:165:GLU:C	2.60	0.43
1:B:270:GLY:HA2	1:B:273:ARG:CD	2.49	0.43
1:B:316:ASP:OD1	1:B:316:ASP:N	2.45	0.43
1:B:326:VAL:HG21	1:B:350:GLU:HG3	2.01	0.43
1:A:24:ALA:O	1:A:25:ASN:C	2.60	0.43
1:A:245:LEU:HG	1:A:249:LEU:CD1	2.43	0.43
1:A:262:ALA:O	1:A:263:ALA:C	2.60	0.43
1:A:287:PHE:CD1	1:A:287:PHE:C	2.95	0.43
1:B:12:VAL:HG12	1:B:108:ARG:HB2	1.99	0.43
1:B:249:LEU:C	1:B:251:GLU:H	2.24	0.43
1:A:158:ARG:O	1:A:161:LEU:HB2	2.18	0.43
1:A:20:ALA:HA	1:A:23:ARG:HB3	2.00	0.43
1:A:207:VAL:CG2	1:A:274:LEU:CD1	2.97	0.43
1:B:93:PHE:O	1:B:94:LEU:C	2.62	0.43
1:B:158:ARG:HD2	1:B:159:GLU:HB2	2.01	0.43
1:A:51:TYR:O	1:A:52:ALA:C	2.60	0.43
1:B:105:HIS:C	1:B:105:HIS:CD2	2.96	0.43
1:B:242:SER:O	1:B:242:SER:OG	2.33	0.43
1:B:327:ILE:HD13	1:B:332:LEU:HB2	1.99	0.43
1:A:262:ALA:C	1:A:265:GLY:H	2.23	0.43
1:B:273:ARG:HH11	1:B:273:ARG:CG	2.32	0.43
1:A:71:VAL:HG21	1:A:275:ALA:O	2.19	0.43
1:A:157:ASP:OD2	1:A:159:GLU:N	2.52	0.43
1:A:160:ARG:HH12	1:A:163:LEU:HD22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASN:OD1	1:B:42:VAL:HG22	2.19	0.43
1:B:212:GLU:CG	1:B:244:ARG:HD3	2.49	0.43
1:B:179:PRO:HB2	1:B:181:ARG:HG2	2.01	0.42
1:B:249:LEU:O	1:B:250:ALA:C	2.60	0.42
1:B:252:LEU:HD12	1:B:260:LEU:HD23	2.00	0.42
1:A:51:TYR:HB2	1:B:55:ARG:NH2	2.33	0.42
1:B:50:LEU:HD21	1:B:297:ALA:HB2	1.99	0.42
1:B:216:PRO:O	1:B:273:ARG:NH2	2.52	0.42
1:B:299:THR:CG2	1:B:300:VAL:N	2.82	0.42
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.79	0.42
1:A:179:PRO:HB2	1:A:181:ARG:HG2	2.01	0.42
1:A:181:ARG:NH2	1:A:204:VAL:CG2	2.82	0.42
1:A:242:SER:O	1:A:243:ALA:C	2.62	0.42
1:A:242:SER:O	1:A:246:GLU:HB2	2.19	0.42
1:B:362:ILE:CG2	1:B:363:TYR:N	2.82	0.42
1:B:175:GLN:OE1	1:B:175:GLN:HA	2.19	0.42
1:B:357:GLN:O	1:B:358:ASP:C	2.62	0.42
1:A:55:ARG:CZ	1:B:51:TYR:HB3	2.50	0.42
1:A:245:LEU:CG	1:A:249:LEU:HD11	2.44	0.42
1:B:14:LYS:NZ	1:B:77:ALA:HB2	2.18	0.42
1:A:54:GLN:CG	1:A:63:VAL:HG22	2.48	0.42
1:B:214:ASP:O	1:B:218:GLY:CA	2.68	0.42
1:B:301:ARG:O	1:B:304:THR:OG1	2.30	0.42
1:B:97:ILE:CG2	1:B:199:LEU:HD13	2.50	0.42
1:B:131:VAL:O	1:B:135:LEU:HD12	2.20	0.42
1:B:146:ARG:HA	1:B:146:ARG:HD2	1.60	0.42
1:B:155:ARG:C	1:B:157:ASP:N	2.73	0.42
1:B:213:GLU:CD	1:B:213:GLU:N	2.76	0.42
1:B:226:ALA:O	1:B:230:LYS:N	2.47	0.42
1:B:268:GLU:HG3	1:B:272:GLN:HB2	2.02	0.42
1:B:295:VAL:O	1:B:295:VAL:CG1	2.68	0.42
1:A:255:GLU:HA	1:A:258:ARG:HB2	2.02	0.41
1:A:342:LYS:HG3	1:A:347:VAL:HG21	2.02	0.41
1:A:16:THR:HB	1:A:243:ALA:CB	2.27	0.41
1:A:75:ASP:O	1:A:76:ILE:C	2.62	0.41
1:A:112:ASP:HB2	1:A:113:PRO:HD2	2.01	0.41
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.82	0.41
1:B:123:ASP:OD2	1:B:123:ASP:C	2.63	0.41
1:A:77:ALA:O	1:A:80:VAL:N	2.53	0.41
1:A:325:GLU:OE1	1:A:342:LYS:NZ	2.50	0.41
1:A:340:ARG:HH11	1:A:340:ARG:HD2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLY:C	1:B:313:ILE:H	2.26	0.41
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.87	0.41
1:A:140:LEU:O	1:A:141:ALA:C	2.61	0.41
1:A:139:ASP:O	1:A:142:THR:HB	2.21	0.41
1:A:328:PRO:O	1:A:329:TRP:C	2.63	0.41
1:B:151:ARG:HA	1:B:164:LEU:CD1	2.51	0.41
1:B:271:LEU:HD12	1:B:271:LEU:H	1.84	0.41
1:B:15:SER:C	1:B:17:LEU:N	2.78	0.41
1:B:71:VAL:HB	1:B:73:PHE:HE1	1.84	0.41
1:B:287:PHE:CD1	1:B:287:PHE:C	2.97	0.41
1:B:307:PRO:O	1:B:310:ALA:N	2.51	0.41
1:B:268:GLU:HG3	1:B:272:GLN:CB	2.51	0.41
1:A:20:ALA:O	1:A:23:ARG:N	2.53	0.41
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.89	0.41
1:B:19:ASN:C	1:B:19:ASN:HD22	2.28	0.41
1:B:23:ARG:HH21	1:B:251:GLU:CG	2.33	0.41
1:B:63:VAL:HA	1:B:64:PRO:HD3	1.92	0.41
1:A:207:VAL:HG21	1:A:274:LEU:CD1	2.51	0.40
1:B:280:ARG:CG	1:B:280:ARG:NH1	2.83	0.40
1:B:328:PRO:HB2	1:B:330:ASP:OD1	2.21	0.40
1:A:48:GLU:OE1	1:B:55:ARG:NH2	2.54	0.40
1:A:76:ILE:HD13	1:A:76:ILE:HA	1.81	0.40
1:A:163:LEU:HD11	1:A:191:ARG:NH2	2.36	0.40
1:A:282:LEU:HB2	1:A:284:LEU:HG	2.04	0.40
1:B:206:TYR:O	1:B:208:ALA:N	2.52	0.40
1:B:270:GLY:HA2	1:B:273:ARG:HD3	2.03	0.40
1:A:136:LEU:HD23	1:A:136:LEU:HA	1.72	0.40
1:A:146:ARG:HA	1:A:146:ARG:HD2	1.68	0.40
1:A:147:LEU:O	1:A:148:GLU:C	2.64	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	348/368 (95%)	286 (82%)	48 (14%)	14 (4%)	2	5
1	B	329/368 (89%)	264 (80%)	46 (14%)	19 (6%)	1	2
All	All	677/736 (92%)	550 (81%)	94 (14%)	33 (5%)	1	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	82	GLY
1	A	189	VAL
1	A	352	LYS
1	B	10	PRO
1	B	79	LEU
1	B	100	VAL
1	B	189	VAL
1	A	56	THR
1	A	188	ALA
1	B	14	LYS
1	B	253	SER
1	B	315	SER
1	B	356	VAL
1	B	151	ARG
1	B	255	GLU
1	B	16	THR
1	B	207	VAL
1	B	258	ARG
1	A	38	LYS
1	A	83	ALA
1	A	263	ALA
1	B	221	ASN
1	B	248	GLU
1	B	262	ALA
1	B	312	GLU
1	B	156	ALA
1	A	111	PRO
1	A	86	GLY
1	A	130	VAL
1	A	241	VAL
1	A	222	PRO
1	B	130	VAL

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	277/289 (96%)	241 (87%)	36 (13%)	4	12
1	B	266/289 (92%)	226 (85%)	40 (15%)	3	8
All	All	543/578 (94%)	467 (86%)	76 (14%)	3	10

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ILE
1	A	9	LEU
1	A	12	VAL
1	A	42	VAL
1	A	44	PRO
1	A	45	LEU
1	A	46	GLU
1	A	74	VAL
1	A	84	HIS
1	A	97	ILE
1	A	112	ASP
1	A	113	PRO
1	A	125	LEU
1	A	150	LEU
1	A	151	ARG
1	A	152	LYS
1	A	212	GLU
1	A	213	GLU
1	A	217	ASP
1	A	230	LYS
1	A	240	VAL
1	A	244	ARG
1	A	268	GLU
1	A	273	ARG
1	A	274	LEU
1	A	276	ARG

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Mol	Chain	Res	Type
1	A	286	THR
1	A	288	PHE
1	A	299	THR
1	A	301	ARG
1	A	302	ARG
1	A	319	ARG
1	A	325	GLU
1	A	340	ARG
1	A	349	LEU
1	B	6	ILE
1	B	7	VAL
1	B	10	PRO
1	B	12	VAL
1	B	21	LEU
1	B	25	ASN
1	B	63	VAL
1	B	74	VAL
1	B	80	VAL
1	B	92	GLN
1	B	94	LEU
1	B	110	PHE
1	B	125	LEU
1	B	127	ASP
1	B	132	GLU
1	B	146	ARG
1	B	150	LEU
1	B	155	ARG
1	B	163	LEU
1	B	174	LEU
1	B	182	THR
1	B	199	LEU
1	B	213	GLU
1	B	217	ASP
1	B	242	SER
1	B	249	LEU
1	B	251	GLU
1	B	258	ARG
1	B	259	GLU
1	B	273	ARG
1	B	280	ARG
1	B	287	PHE
1	B	293	LYS

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Mol	Chain	Res	Type
1	B	294	GLU
1	B	295	VAL
1	B	317	MET
1	B	340	ARG
1	B	352	LYS
1	B	356	VAL
1	B	364	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	92	GLN
1	A	223	GLN
1	A	357	GLN
1	A	367	ASN
1	B	11	ASN
1	B	19	ASN
1	B	54	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	354/368 (96%)	-0.43	2 (0%) 85 82	14, 49, 90, 119	1 (0%)
1	B	337/368 (91%)	-0.22	2 (0%) 85 82	8, 65, 108, 145	1 (0%)
All	All	691/736 (93%)	-0.33	4 (0%) 85 82	8, 56, 100, 145	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	ARG	2.6
1	B	368	ALA	2.4
1	B	271	LEU	2.1
1	A	368	ALA	2.1

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.