



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:09 AM UTC

PDB ID : 3RFY / pdb_00003rfy
Title : Crystal structure of arabidopsis thaliana cyclophilin 38 (ATCYP38)
Authors : Vasudevan, D.; Swaminathan, K.
Deposited on : 2011-04-07
Resolution : 2.39 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

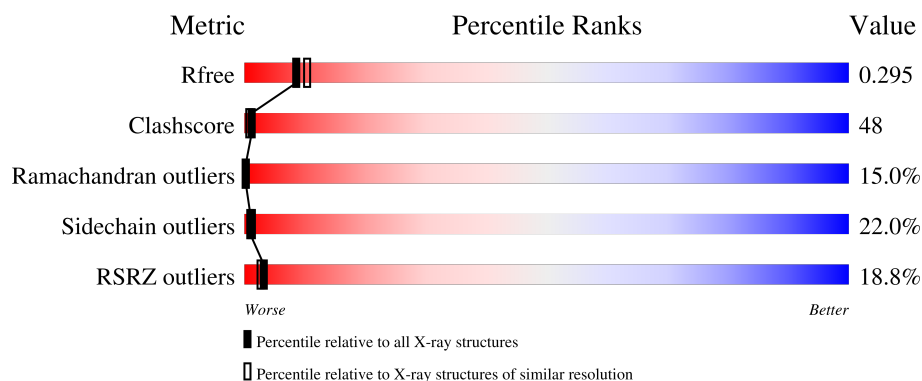
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	369	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2879 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 Peptidyl-prolyl cis-trans isomerase CYP38, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2765	1751	456	547	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLY	-	expression tag	UNP Q9SSA5
A	70	SER	-	expression tag	UNP Q9SSA5
A	71	PRO	-	expression tag	UNP Q9SSA5
A	72	GLY	-	expression tag	UNP Q9SSA5
A	73	ILE	-	expression tag	UNP Q9SSA5
A	74	SER	-	expression tag	UNP Q9SSA5
A	75	GLY	-	expression tag	UNP Q9SSA5
A	76	GLY	-	expression tag	UNP Q9SSA5
A	77	GLY	-	expression tag	UNP Q9SSA5
A	78	GLY	-	expression tag	UNP Q9SSA5
A	79	GLY	-	expression tag	UNP Q9SSA5
A	80	ILE	-	expression tag	UNP Q9SSA5
A	81	LEU	-	expression tag	UNP Q9SSA5
A	82	LEU	-	expression tag	UNP Q9SSA5

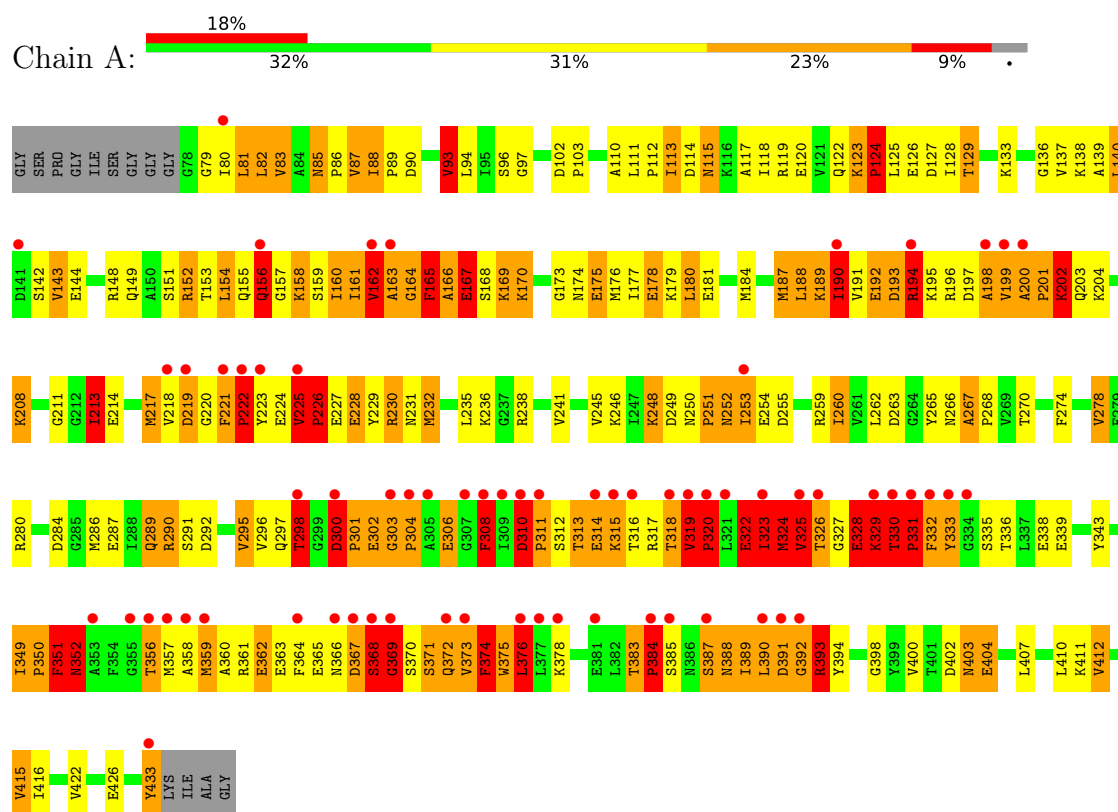
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		

3 Residue-property plots [i](#)

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: Peptidyl-prolyl cis-trans isomerase CYP38, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	57.69Å 96.72Å 166.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.39 19.89 – 2.39	Depositor EDS
% Data completeness (in resolution range)	86.9 (19.89-2.39) 86.7 (19.89-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.266 0.256 , 0.295	Depositor DCC
R_{free} test set	836 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.043 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2879	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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	0.99	4/2814 (0.1%)	1.84	104/3810 (2.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	TRP	NE1-CE2	11.35	1.50	1.37
1	A	329	LYS	CA-C	7.01	1.62	1.52
1	A	330	THR	CA-C	6.00	1.60	1.52
1	A	329	LYS	N-CA	5.21	1.52	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	LYS	N-CA-C	-16.45	92.44	113.17
1	A	191	VAL	N-CA-C	-15.36	93.78	112.98
1	A	88	ILE	CA-C-N	14.73	138.25	119.84
1	A	88	ILE	C-N-CA	14.73	138.25	119.84
1	A	298	THR	N-CA-C	14.30	128.63	111.33
1	A	200	ALA	CA-C-N	-14.17	102.13	119.84
1	A	200	ALA	C-N-CA	-14.17	102.13	119.84
1	A	388	ASN	N-CA-C	12.56	129.62	110.14
1	A	165	PHE	N-CA-C	12.42	128.49	112.34
1	A	387	SER	N-CA-C	11.88	125.80	108.34
1	A	81	LEU	N-CA-C	11.59	128.27	109.72
1	A	123	LYS	CA-C-N	-11.28	105.75	119.84
1	A	123	LYS	C-N-CA	-11.28	105.75	119.84
1	A	371	SER	N-CA-C	11.11	124.66	110.33
1	A	297	GLN	N-CA-C	-11.06	87.71	108.17
1	A	227	GLU	N-CA-C	10.04	126.11	111.96
1	A	372	GLN	N-CA-C	9.61	131.26	110.80
1	A	194	ARG	N-CA-C	-9.52	90.52	110.80
1	A	391	ASP	N-CA-C	9.32	130.66	110.80
1	A	375	TRP	CD2-CE2-CZ2	9.28	131.68	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASN	CA-C-N	-8.74	108.91	119.84
1	A	85	ASN	C-N-CA	-8.74	108.91	119.84
1	A	306	GLU	N-CA-C	8.68	122.26	110.55
1	A	367	ASP	N-CA-C	8.10	128.06	110.80
1	A	164	GLY	N-CA-C	8.02	132.19	113.18
1	A	416	ILE	CB-CA-C	-7.83	102.77	111.23
1	A	356	THR	N-CA-C	7.61	121.88	109.85
1	A	297	GLN	CA-C-N	7.59	130.78	120.38
1	A	297	GLN	C-N-CA	7.59	130.78	120.38
1	A	175	GLU	N-CA-C	-7.54	103.07	111.82
1	A	325	VAL	N-CA-C	7.54	125.02	109.34
1	A	374	PHE	N-CA-C	7.43	126.62	110.80
1	A	415	VAL	N-CA-C	7.39	118.51	108.17
1	A	251	PRO	N-CA-C	-7.37	97.17	111.69
1	A	383	THR	N-CA-C	-7.34	100.84	110.39
1	A	226	PRO	N-CA-C	7.29	121.42	111.22
1	A	208	LYS	N-CA-C	-7.26	103.44	111.36
1	A	219	ASP	N-CA-C	-7.25	95.35	110.80
1	A	324	MET	N-CA-C	7.20	126.14	110.80
1	A	160	ILE	N-CA-C	-7.19	104.19	110.74
1	A	166	ALA	N-CA-C	7.12	125.97	110.80
1	A	390	LEU	N-CA-C	7.11	119.98	108.76
1	A	156	GLN	N-CA-C	-7.01	95.86	110.80
1	A	300	ASP	N-CA-C	6.99	125.25	109.81
1	A	223	TYR	N-CA-C	-6.85	103.74	111.14
1	A	267	ALA	CA-C-N	6.76	126.27	119.24
1	A	267	ALA	C-N-CA	6.76	126.27	119.24
1	A	328	GLU	N-CA-C	6.74	121.73	108.18
1	A	331	PRO	N-CA-C	6.74	126.35	112.47
1	A	358	ALA	N-CA-C	6.70	125.07	110.80
1	A	319	VAL	N-CA-C	-6.69	94.44	108.88
1	A	375	TRP	CE2-CD2-CG	6.53	115.04	107.20
1	A	232	MET	N-CA-C	-6.48	102.53	110.31
1	A	375	TRP	N-CA-C	6.46	117.65	108.74
1	A	289	GLN	N-CA-C	-6.45	99.40	109.72
1	A	375	TRP	CE2-CD2-CE3	-6.44	112.36	118.80
1	A	349	ILE	CA-C-N	6.42	127.87	119.84
1	A	349	ILE	C-N-CA	6.42	127.87	119.84
1	A	93	VAL	N-CA-C	6.42	117.53	108.36
1	A	190	ILE	N-CA-C	-6.37	96.09	109.34
1	A	329	LYS	N-CA-C	6.35	124.33	110.80
1	A	393	ARG	N-CA-C	6.34	124.32	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ASP	CB-CA-C	-6.34	102.61	112.31
1	A	352	ASN	N-CA-C	6.32	124.25	110.80
1	A	97	GLY	CA-C-N	6.18	126.74	120.38
1	A	97	GLY	C-N-CA	6.18	126.74	120.38
1	A	213	ILE	CB-CA-C	-6.17	104.07	111.97
1	A	195	LYS	N-CA-C	-6.17	97.67	110.80
1	A	336	THR	N-CA-C	-6.13	99.98	109.24
1	A	322	GLU	N-CA-C	6.12	123.84	110.80
1	A	416	ILE	N-CA-C	-6.04	98.86	107.98
1	A	370	SER	N-CA-C	5.98	123.54	110.80
1	A	278	VAL	N-CA-C	-5.94	104.72	110.72
1	A	387	SER	CB-CA-C	-5.87	107.97	116.54
1	A	263	ASP	N-CA-C	5.72	118.67	107.57
1	A	303	GLY	N-CA-C	5.68	123.92	112.34
1	A	222	PRO	N-CA-C	5.64	124.09	112.47
1	A	301	PRO	N-CA-C	5.57	123.94	112.47
1	A	225	VAL	CA-C-N	5.52	125.51	120.21
1	A	225	VAL	C-N-CA	5.52	125.51	120.21
1	A	311	PRO	N-CA-C	5.44	123.67	112.47
1	A	284	ASP	N-CA-C	5.43	118.11	109.96
1	A	369	GLY	N-CA-C	5.43	126.06	113.18
1	A	433	TYR	N-CA-C	5.41	126.16	111.00
1	A	313	THR	N-CA-C	5.39	117.17	109.14
1	A	422	VAL	CB-CA-C	5.38	115.92	110.65
1	A	388	ASN	CA-C-N	5.37	131.64	121.97
1	A	388	ASN	C-N-CA	5.37	131.64	121.97
1	A	211	GLY	N-CA-C	-5.33	106.31	112.50
1	A	383	THR	CA-C-N	-5.32	113.19	119.84
1	A	383	THR	C-N-CA	-5.32	113.19	119.84
1	A	390	LEU	CA-C-N	5.25	131.58	121.54
1	A	390	LEU	C-N-CA	5.25	131.58	121.54
1	A	376	LEU	N-CA-C	5.25	121.99	110.80
1	A	295	VAL	N-CA-CB	-5.25	105.06	111.67
1	A	308	PHE	N-CA-C	5.24	117.94	110.24
1	A	362	GLU	N-CA-C	5.19	121.86	110.80
1	A	124	PRO	N-CA-C	-5.19	101.78	112.47
1	A	412	VAL	N-CA-C	-5.14	102.23	109.63
1	A	403	ASN	N-CA-C	-5.09	107.02	113.23
1	A	323	ILE	CA-C-N	5.07	131.22	121.54
1	A	323	ILE	C-N-CA	5.07	131.22	121.54
1	A	302	GLU	N-CA-C	5.03	121.51	110.80
1	A	248	LYS	N-CA-C	5.01	117.94	110.52

There are no chirality outliers.

There are no planarity outliers.

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	2765	0	2753	264	1
2	A	114	0	0	30	2
All	All	2879	0	2753	264	2

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 48.

All (264) 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:A:319:VAL:H	1:A:320:PRO:CD	1.60	1.10
1:A:88:ILE:N	1:A:89:PRO:HD3	1.56	1.10
1:A:86:PRO:HB2	2:A:684:HOH:O	1.53	1.08
1:A:129:THR:HG22	1:A:203:GLN:HE22	1.12	1.08
1:A:319:VAL:H	1:A:320:PRO:HD2	1.19	1.06
1:A:260:ILE:HD13	1:A:400:VAL:HG22	1.38	1.02
1:A:158:LYS:O	1:A:162:VAL:HG23	1.58	1.01
1:A:157:GLY:HA3	2:A:674:HOH:O	1.63	0.98
1:A:308:PHE:HD1	1:A:308:PHE:H	1.10	0.98
1:A:187:MET:HE1	1:A:200:ALA:HA	1.45	0.97
1:A:80:ILE:HG23	1:A:96:SER:HB3	1.48	0.96
1:A:80:ILE:HD12	1:A:96:SER:HB2	1.47	0.96
1:A:125:LEU:N	2:A:671:HOH:O	1.98	0.96
1:A:280:ARG:HD3	2:A:683:HOH:O	1.64	0.95
1:A:80:ILE:HG21	1:A:407:LEU:CD1	1.98	0.93
1:A:88:ILE:N	1:A:89:PRO:CD	2.31	0.92
1:A:79:GLY:O	1:A:80:ILE:HD13	1.73	0.89
1:A:221:PHE:HB3	1:A:222:PRO:HD2	1.54	0.88
1:A:319:VAL:N	1:A:320:PRO:CD	2.36	0.88
1:A:169:LYS:HD3	1:A:219:ASP:OD2	1.73	0.88
1:A:218:VAL:HG21	2:A:670:HOH:O	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:O	1:A:315:LYS:HB2	1.71	0.87
1:A:190:ILE:HD11	1:A:199:VAL:CG1	2.05	0.86
1:A:330:THR:HG22	1:A:331:PRO:HD2	1.58	0.86
1:A:331:PRO:O	1:A:332:PHE:O	1.94	0.85
1:A:80:ILE:HB	1:A:400:VAL:HB	1.56	0.85
1:A:200:ALA:O	1:A:202:LYS:N	2.11	0.83
1:A:113:ILE:HD11	1:A:214:GLU:O	1.77	0.83
1:A:169:LYS:CD	1:A:219:ASP:OD2	2.27	0.83
1:A:129:THR:CG2	1:A:203:GLN:HE22	1.93	0.82
1:A:189:LYS:O	1:A:190:ILE:HG13	1.79	0.82
1:A:190:ILE:HA	1:A:192:GLU:HG2	1.61	0.82
1:A:80:ILE:HG21	1:A:407:LEU:HD13	1.63	0.81
1:A:129:THR:HG22	1:A:203:GLN:NE2	1.96	0.81
1:A:80:ILE:HG21	1:A:407:LEU:HD11	1.63	0.80
1:A:154:LEU:O	1:A:156:GLN:N	2.14	0.80
1:A:330:THR:CG2	1:A:331:PRO:HD2	2.12	0.79
1:A:159:SER:O	1:A:163:ALA:HB3	1.82	0.78
1:A:426:GLU:OE1	2:A:654:HOH:O	2.03	0.76
1:A:221:PHE:HB3	1:A:222:PRO:CD	2.15	0.76
1:A:177:ILE:O	1:A:181:GLU:HG3	1.86	0.76
1:A:80:ILE:HG23	1:A:96:SER:CB	2.16	0.76
1:A:87:VAL:C	1:A:89:PRO:HD3	2.11	0.75
1:A:140:LEU:N	1:A:140:LEU:HD12	2.00	0.75
1:A:80:ILE:CD1	1:A:96:SER:HB2	2.17	0.75
1:A:350:PRO:HB2	1:A:352:ASN:HD21	1.53	0.74
1:A:190:ILE:HD11	1:A:199:VAL:CB	2.17	0.74
1:A:389:ILE:O	1:A:390:LEU:HD22	1.87	0.74
1:A:426:GLU:OE1	2:A:605:HOH:O	2.04	0.74
1:A:190:ILE:HD11	1:A:199:VAL:HB	1.69	0.73
1:A:350:PRO:O	1:A:351:PHE:HB2	1.87	0.73
1:A:80:ILE:CG2	1:A:407:LEU:HD13	2.19	0.73
1:A:319:VAL:N	1:A:320:PRO:HD2	2.00	0.73
1:A:280:ARG:HB2	1:A:433:TYR:CG	2.24	0.73
1:A:350:PRO:O	1:A:351:PHE:CB	2.36	0.72
1:A:286:MET:HE3	1:A:350:PRO:HA	1.70	0.72
1:A:248:LYS:O	1:A:411:LYS:NZ	2.23	0.72
1:A:378:LYS:NZ	2:A:641:HOH:O	2.23	0.71
1:A:378:LYS:HE3	2:A:641:HOH:O	1.89	0.71
1:A:162:VAL:O	1:A:163:ALA:C	2.34	0.71
1:A:126:GLU:O	1:A:129:THR:HG23	1.90	0.70
1:A:86:PRO:C	1:A:88:ILE:H	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:O	1:A:179:LYS:HG3	1.91	0.70
1:A:290:ARG:NH2	1:A:292:ASP:OD1	2.25	0.69
1:A:378:LYS:CE	2:A:641:HOH:O	2.40	0.69
1:A:83:VAL:HG12	1:A:93:VAL:HB	1.74	0.69
1:A:327:GLY:C	1:A:328:GLU:HG2	2.17	0.68
1:A:199:VAL:O	1:A:202:LYS:HB3	1.94	0.68
1:A:313:THR:O	1:A:314:GLU:HB2	1.93	0.68
1:A:113:ILE:HG13	1:A:218:VAL:HB	1.75	0.67
1:A:144:GLU:OE1	1:A:148:ARG:NH1	2.27	0.67
1:A:190:ILE:C	1:A:192:GLU:H	1.93	0.67
1:A:392:GLY:O	1:A:393:ARG:HB2	1.94	0.67
1:A:308:PHE:N	1:A:308:PHE:CD1	2.62	0.67
1:A:222:PRO:HG2	1:A:236:LYS:HG2	1.76	0.67
1:A:225:VAL:HG12	1:A:226:PRO:HD2	1.75	0.67
1:A:289:GLN:NE2	1:A:349:ILE:HD11	2.09	0.67
1:A:287:GLU:O	1:A:350:PRO:O	2.13	0.67
1:A:322:GLU:HB3	1:A:324:MET:H	1.59	0.67
1:A:190:ILE:C	1:A:192:GLU:N	2.48	0.67
1:A:190:ILE:CA	1:A:192:GLU:HG2	2.24	0.67
1:A:140:LEU:HD12	1:A:140:LEU:H	1.58	0.67
1:A:251:PRO:O	1:A:252:ASN:HB2	1.94	0.66
1:A:252:ASN:O	1:A:253:ILE:HG22	1.96	0.66
1:A:190:ILE:HA	1:A:192:GLU:CG	2.26	0.66
1:A:123:LYS:C	1:A:124:PRO:O	2.38	0.65
1:A:178:GLU:HG2	2:A:628:HOH:O	1.97	0.65
1:A:129:THR:HB	2:A:692:HOH:O	1.97	0.64
1:A:124:PRO:O	1:A:126:GLU:N	2.29	0.64
1:A:289:GLN:HE22	1:A:349:ILE:HD11	1.62	0.64
1:A:122:GLN:O	1:A:124:PRO:O	2.16	0.63
1:A:176:MET:HB3	1:A:213:ILE:HD13	1.80	0.63
1:A:350:PRO:HB2	1:A:352:ASN:ND2	2.12	0.63
1:A:87:VAL:C	1:A:89:PRO:CD	2.70	0.63
1:A:140:LEU:H	1:A:140:LEU:CD1	2.11	0.63
1:A:349:ILE:HB	1:A:350:PRO:HD2	1.79	0.63
1:A:310:ASP:HB3	1:A:311:PRO:CD	2.29	0.62
1:A:296:VAL:HG21	1:A:378:LYS:HD2	1.81	0.62
1:A:115:ASN:HD21	1:A:117:ALA:HB3	1.65	0.62
1:A:89:PRO:O	1:A:90:ASP:HB2	1.97	0.62
1:A:280:ARG:HB2	1:A:433:TYR:CD2	2.35	0.62
1:A:88:ILE:H	1:A:89:PRO:HD3	1.58	0.61
1:A:113:ILE:CD1	1:A:214:GLU:O	2.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:SER:OG	1:A:388:ASN:N	2.33	0.61
1:A:80:ILE:CG2	1:A:407:LEU:CD1	2.72	0.61
1:A:200:ALA:C	1:A:202:LYS:H	2.07	0.60
1:A:251:PRO:O	1:A:252:ASN:CB	2.48	0.60
1:A:222:PRO:HG3	2:A:604:HOH:O	2.01	0.59
1:A:280:ARG:HG2	2:A:643:HOH:O	2.01	0.59
1:A:260:ILE:CD1	1:A:400:VAL:HG22	2.22	0.59
1:A:115:ASN:C	1:A:115:ASN:HD22	2.12	0.58
1:A:157:GLY:O	1:A:161:ILE:HG13	2.03	0.58
1:A:88:ILE:O	1:A:88:ILE:HG22	2.02	0.58
1:A:103:PRO:HG3	1:A:404:GLU:OE2	2.04	0.58
1:A:349:ILE:HB	1:A:350:PRO:CD	2.33	0.58
1:A:140:LEU:N	1:A:140:LEU:CD1	2.67	0.58
1:A:119:ARG:HH11	1:A:122:GLN:HE22	1.50	0.58
1:A:266:ASN:O	1:A:384:PRO:HD2	2.04	0.58
1:A:296:VAL:CG2	1:A:378:LYS:HD2	2.34	0.58
1:A:220:GLY:N	2:A:707:HOH:O	2.33	0.58
1:A:319:VAL:O	1:A:324:MET:HE3	2.03	0.58
1:A:192:GLU:O	1:A:193:ASP:C	2.48	0.57
1:A:238:ARG:HH11	1:A:265:TYR:HD1	1.52	0.57
1:A:359:MET:HG2	1:A:360:ALA:H	1.69	0.56
1:A:79:GLY:C	1:A:80:ILE:HD13	2.30	0.56
1:A:198:ALA:O	1:A:199:VAL:HG23	2.05	0.56
1:A:189:LYS:O	1:A:190:ILE:CG1	2.53	0.56
1:A:80:ILE:HG13	1:A:407:LEU:CD1	2.36	0.56
1:A:164:GLY:HA3	2:A:611:HOH:O	2.06	0.56
1:A:120:GLU:O	1:A:124:PRO:HD2	2.06	0.55
1:A:300:ASP:OD1	2:A:610:HOH:O	2.18	0.55
1:A:161:ILE:HD13	1:A:174:ASN:OD1	2.07	0.55
1:A:426:GLU:CD	2:A:605:HOH:O	2.48	0.55
1:A:193:ASP:O	1:A:194:ARG:HB2	2.05	0.54
1:A:254:GLU:HA	2:A:703:HOH:O	2.05	0.54
1:A:200:ALA:C	1:A:202:LYS:N	2.65	0.54
1:A:196:ARG:HG2	1:A:196:ARG:O	2.08	0.54
1:A:123:LYS:HE3	1:A:127:ASP:OD2	2.08	0.54
1:A:153:THR:O	1:A:156:GLN:HB3	2.07	0.54
1:A:221:PHE:CB	1:A:222:PRO:HD2	2.33	0.54
1:A:124:PRO:O	1:A:125:LEU:HB2	2.08	0.54
1:A:323:ILE:O	1:A:323:ILE:CG2	2.55	0.53
1:A:176:MET:CB	1:A:213:ILE:HD13	2.37	0.53
1:A:86:PRO:C	1:A:88:ILE:N	2.65	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:O	1:A:385:SER:N	2.42	0.53
1:A:165:PHE:HB3	1:A:170:LYS:HG2	1.91	0.53
1:A:136:GLY:O	1:A:138:LYS:N	2.42	0.52
1:A:213:ILE:HG22	1:A:217:MET:HE3	1.91	0.52
1:A:225:VAL:HG12	1:A:226:PRO:CD	2.38	0.52
1:A:81:LEU:O	1:A:94:LEU:HA	2.08	0.52
1:A:266:ASN:C	1:A:268:PRO:HD3	2.35	0.52
1:A:296:VAL:C	1:A:298:THR:N	2.66	0.52
1:A:359:MET:HG2	1:A:360:ALA:N	2.25	0.52
1:A:89:PRO:O	1:A:90:ASP:CB	2.58	0.52
1:A:124:PRO:C	1:A:126:GLU:H	2.18	0.52
1:A:245:VAL:O	1:A:255:ASP:HB2	2.10	0.52
1:A:289:GLN:OE1	1:A:351:PHE:HA	2.10	0.52
1:A:124:PRO:C	1:A:126:GLU:N	2.67	0.52
1:A:83:VAL:HG13	1:A:394:TYR:CD2	2.45	0.51
1:A:201:PRO:HB2	2:A:609:HOH:O	2.09	0.51
1:A:349:ILE:HD12	2:A:679:HOH:O	2.10	0.51
1:A:260:ILE:HD13	1:A:400:VAL:CG2	2.27	0.51
1:A:290:ARG:H	1:A:412:VAL:HG12	1.74	0.51
1:A:322:GLU:O	1:A:323:ILE:HB	2.10	0.51
1:A:267:ALA:N	1:A:268:PRO:HD3	2.26	0.50
1:A:328:GLU:O	1:A:329:LYS:HB2	2.11	0.50
1:A:204:LYS:O	1:A:208:LYS:HG2	2.11	0.50
1:A:402:ASP:O	1:A:403:ASN:HB2	2.11	0.50
1:A:176:MET:CB	1:A:213:ILE:CD1	2.89	0.49
1:A:322:GLU:HG2	1:A:324:MET:HA	1.94	0.49
1:A:139:ALA:O	1:A:142:SER:HB3	2.12	0.49
1:A:114:ASP:OD1	1:A:114:ASP:C	2.56	0.49
1:A:274:PHE:O	1:A:278:VAL:HG23	2.13	0.49
1:A:392:GLY:N	2:A:653:HOH:O	2.35	0.48
1:A:85:ASN:OD1	2:A:669:HOH:O	2.20	0.48
1:A:161:ILE:CD1	1:A:174:ASN:OD1	2.62	0.48
1:A:190:ILE:HD11	1:A:199:VAL:HG11	1.91	0.48
1:A:300:ASP:CB	1:A:301:PRO:CD	2.92	0.47
1:A:140:LEU:HA	1:A:143:VAL:HG13	1.96	0.47
1:A:167:GLU:HB2	1:A:168:SER:H	1.37	0.47
1:A:374:PHE:O	1:A:375:TRP:CD1	2.68	0.47
1:A:80:ILE:CG1	1:A:407:LEU:CD1	2.92	0.47
1:A:160:ILE:HG23	1:A:217:MET:HE2	1.97	0.47
1:A:120:GLU:HB3	1:A:153:THR:HG21	1.95	0.47
1:A:388:ASN:C	1:A:389:ILE:HG13	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ALA:HB3	1:A:201:PRO:HD3	1.97	0.46
1:A:259:ARG:HB3	1:A:402:ASP:HB3	1.97	0.46
1:A:253:ILE:HG23	1:A:253:ILE:O	2.14	0.46
1:A:324:MET:O	1:A:325:VAL:O	2.33	0.46
1:A:152:ARG:CD	2:A:617:HOH:O	2.63	0.46
1:A:102:ASP:HA	1:A:103:PRO:HD2	1.79	0.46
1:A:229:TYR:C	1:A:231:ASN:H	2.24	0.46
1:A:364:PHE:HD1	1:A:364:PHE:O	1.98	0.46
1:A:249:ASP:HB3	2:A:697:HOH:O	2.15	0.46
1:A:176:MET:HB2	1:A:213:ILE:CD1	2.46	0.45
1:A:296:VAL:O	1:A:298:THR:N	2.49	0.45
1:A:388:ASN:O	1:A:389:ILE:HG13	2.16	0.45
1:A:329:LYS:O	1:A:330:THR:O	2.34	0.45
1:A:333:TYR:C	1:A:333:TYR:CD2	2.94	0.45
1:A:115:ASN:ND2	1:A:118:ILE:H	2.15	0.45
1:A:190:ILE:HD11	1:A:199:VAL:HG12	1.94	0.45
1:A:229:TYR:HB3	1:A:232:MET:SD	2.57	0.45
1:A:82:LEU:HB2	1:A:398:GLY:HA3	1.99	0.45
1:A:144:GLU:O	1:A:148:ARG:HG3	2.17	0.45
1:A:176:MET:HB3	1:A:213:ILE:CD1	2.45	0.45
1:A:250:ASN:OD1	1:A:252:ASN:O	2.35	0.45
1:A:318:THR:O	1:A:322:GLU:OE2	2.34	0.45
1:A:180:LEU:O	1:A:184:MET:HG3	2.16	0.44
1:A:221:PHE:CB	1:A:222:PRO:CD	2.88	0.44
1:A:333:TYR:CE2	1:A:339:GLU:OE1	2.70	0.44
1:A:359:MET:CG	1:A:360:ALA:H	2.28	0.44
1:A:253:ILE:O	1:A:253:ILE:CG2	2.66	0.44
1:A:87:VAL:N	1:A:89:PRO:HD3	2.33	0.44
1:A:287:GLU:HG2	1:A:415:VAL:HG22	2.00	0.44
1:A:310:ASP:CB	1:A:311:PRO:CD	2.93	0.44
1:A:169:LYS:HD2	1:A:219:ASP:OD2	2.14	0.44
1:A:123:LYS:O	1:A:124:PRO:O	2.36	0.44
1:A:228:GLU:HB2	2:A:675:HOH:O	2.18	0.44
1:A:200:ALA:HB3	1:A:201:PRO:CD	2.49	0.43
1:A:364:PHE:O	1:A:364:PHE:CD1	2.71	0.43
1:A:368:SER:HB3	1:A:369:GLY:H	1.56	0.43
1:A:302:GLU:HB3	1:A:303:GLY:H	1.41	0.43
1:A:343:TYR:CD1	1:A:343:TYR:N	2.87	0.43
1:A:372:GLN:HG2	1:A:374:PHE:CE1	2.53	0.43
1:A:365:GLU:H	1:A:365:GLU:HG2	1.68	0.43
1:A:136:GLY:C	1:A:138:LYS:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:C	1:A:142:SER:H	2.27	0.43
1:A:188:LEU:HA	1:A:188:LEU:HD22	1.86	0.43
1:A:136:GLY:C	1:A:138:LYS:H	2.27	0.42
1:A:164:GLY:CA	2:A:611:HOH:O	2.66	0.42
1:A:328:GLU:O	1:A:329:LYS:CB	2.66	0.42
1:A:238:ARG:HD3	1:A:265:TYR:CE1	2.54	0.42
1:A:167:GLU:H	1:A:167:GLU:HG3	1.72	0.42
1:A:87:VAL:C	1:A:89:PRO:HD2	2.43	0.42
1:A:111:LEU:HA	1:A:112:PRO:HD3	1.90	0.42
1:A:193:ASP:O	1:A:194:ARG:CB	2.67	0.42
1:A:165:PHE:CZ	1:A:173:GLY:HA3	2.54	0.42
1:A:199:VAL:O	1:A:202:LYS:CB	2.65	0.42
1:A:202:LYS:O	1:A:202:LYS:HG3	2.19	0.42
1:A:246:LYS:NZ	1:A:248:LYS:HE3	2.35	0.42
1:A:280:ARG:CB	1:A:433:TYR:CD2	3.01	0.42
1:A:373:VAL:O	1:A:374:PHE:HB2	2.20	0.42
1:A:188:LEU:O	1:A:190:ILE:N	2.53	0.41
1:A:200:ALA:CB	1:A:201:PRO:HD3	2.50	0.41
1:A:289:GLN:HA	1:A:412:VAL:HG12	2.01	0.41
1:A:290:ARG:O	1:A:291:SER:HB3	2.20	0.41
1:A:118:ILE:HB	1:A:217:MET:HE1	2.03	0.41
1:A:192:GLU:O	1:A:194:ARG:O	2.38	0.41
1:A:349:ILE:CB	1:A:350:PRO:CD	2.98	0.41
1:A:190:ILE:CD1	1:A:199:VAL:HB	2.45	0.41
1:A:326:THR:HG22	1:A:327:GLY:N	2.35	0.41
1:A:338:GLU:HG3	2:A:602:HOH:O	2.19	0.41
1:A:152:ARG:HD2	2:A:617:HOH:O	2.20	0.41
1:A:371:SER:O	1:A:372:GLN:HB2	2.20	0.41
1:A:89:PRO:CG	2:A:687:HOH:O	2.68	0.41
1:A:110:ALA:HB1	1:A:266:ASN:ND2	2.36	0.41
1:A:128:ILE:HG23	1:A:143:VAL:HB	2.03	0.40
1:A:154:LEU:HD12	1:A:184:MET:CE	2.51	0.40
1:A:151:SER:HA	1:A:184:MET:HE1	2.03	0.40
1:A:331:PRO:C	1:A:332:PHE:O	2.62	0.40
1:A:323:ILE:O	1:A:323:ILE:HG22	2.21	0.40
1:A:198:ALA:O	1:A:199:VAL:CG2	2.70	0.40
1:A:245:VAL:HG11	1:A:410:LEU:HD22	2.03	0.40
1:A:280:ARG:HG2	1:A:433:TYR:CD2	2.57	0.40

All (2) 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:605:HOH:O	2:A:605:HOH:O[3_555]	2.15	0.05
1:A:375:TRP:O	2:A:602:HOH:O[4_566]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	354/369 (96%)	257 (73%)	44 (12%)	53 (15%)	0 0

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	A	137	VAL
1	A	155	GLN
1	A	156	GLN
1	A	162	VAL
1	A	163	ALA
1	A	167	GLU
1	A	190	ILE
1	A	217	MET
1	A	222	PRO
1	A	314	GLU
1	A	315	LYS
1	A	320	PRO
1	A	323	ILE
1	A	324	MET
1	A	325	VAL
1	A	329	LYS
1	A	330	THR
1	A	332	PHE
1	A	335	SER
1	A	351	PHE
1	A	363	GLU

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Mol	Chain	Res	Type
1	A	369	GLY
1	A	389	ILE
1	A	391	ASP
1	A	194	ARG
1	A	253	ILE
1	A	300	ASP
1	A	333	TYR
1	A	367	ASP
1	A	374	PHE
1	A	376	LEU
1	A	124	PRO
1	A	199	VAL
1	A	322	GLU
1	A	359	MET
1	A	366	ASN
1	A	393	ARG
1	A	166	ALA
1	A	221	PHE
1	A	230	ARG
1	A	326	THR
1	A	331	PRO
1	A	368	SER
1	A	193	ASP
1	A	198	ALA
1	A	252	ASN
1	A	310	ASP
1	A	319	VAL
1	A	392	GLY
1	A	304	PRO
1	A	373	VAL
1	A	384	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	305/311 (98%)	238 (78%)	67 (22%)	1 1

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	83	VAL
1	A	93	VAL
1	A	113	ILE
1	A	115	ASN
1	A	129	THR
1	A	133	LYS
1	A	140	LEU
1	A	143	VAL
1	A	149	GLN
1	A	152	ARG
1	A	154	LEU
1	A	158	LYS
1	A	161	ILE
1	A	162	VAL
1	A	165	PHE
1	A	167	GLU
1	A	169	LYS
1	A	170	LYS
1	A	178	GLU
1	A	180	LEU
1	A	187	MET
1	A	188	LEU
1	A	189	LYS
1	A	192	GLU
1	A	194	ARG
1	A	201	PRO
1	A	202	LYS
1	A	213	ILE
1	A	222	PRO
1	A	224	GLU
1	A	225	VAL
1	A	226	PRO
1	A	228	GLU
1	A	230	ARG

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Mol	Chain	Res	Type
1	A	235	LEU
1	A	241	VAL
1	A	260	ILE
1	A	262	LEU
1	A	270	THR
1	A	290	ARG
1	A	295	VAL
1	A	298	THR
1	A	304	PRO
1	A	306	GLU
1	A	308	PHE
1	A	310	ASP
1	A	312	SER
1	A	316	THR
1	A	317	ARG
1	A	318	THR
1	A	320	PRO
1	A	322	GLU
1	A	323	ILE
1	A	325	VAL
1	A	328	GLU
1	A	350	PRO
1	A	351	PHE
1	A	352	ASN
1	A	356	THR
1	A	357	MET
1	A	361	ARG
1	A	362	GLU
1	A	368	SER
1	A	376	LEU
1	A	384	PRO
1	A	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	122	GLN
1	A	156	GLN
1	A	185	GLN
1	A	203	GLN
1	A	273	ASN

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Mol	Chain	Res	Type
1	A	289	GLN
1	A	352	ASN
1	A	388	ASN
1	A	403	ASN

5.3.3 RNA [i](#)

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	356/369 (96%)	0.87	67 (18%) 3 3	31, 58, 148, 168	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	LEU	5.9
1	A	330	THR	5.5
1	A	198	ALA	5.0
1	A	373	VAL	4.9
1	A	316	THR	4.7
1	A	309	ILE	4.7
1	A	358	ALA	4.3
1	A	323	ILE	4.3
1	A	218	VAL	4.2
1	A	331	PRO	3.9
1	A	319	VAL	3.9
1	A	366	ASN	3.9
1	A	325	VAL	3.8
1	A	357	MET	3.7
1	A	308	PHE	3.6
1	A	199	VAL	3.6
1	A	329	LYS	3.5
1	A	310	ASP	3.5
1	A	163	ALA	3.4
1	A	332	PHE	3.4
1	A	304	PRO	3.3
1	A	433	TYR	3.2
1	A	80	ILE	3.2
1	A	381	GLU	3.2
1	A	318	THR	3.1
1	A	162	VAL	3.1
1	A	320	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	298	THR	3.0
1	A	326	THR	3.0
1	A	390	LEU	2.9
1	A	356	THR	2.9
1	A	307	GLY	2.9
1	A	221	PHE	2.9
1	A	385	SER	2.9
1	A	378	LYS	2.8
1	A	353	ALA	2.7
1	A	367	ASP	2.7
1	A	368	SER	2.7
1	A	200	ALA	2.7
1	A	223	TYR	2.6
1	A	333	TYR	2.6
1	A	334	GLY	2.6
1	A	300	ASP	2.6
1	A	303	GLY	2.6
1	A	311	PRO	2.6
1	A	387	SER	2.5
1	A	384	PRO	2.5
1	A	305	ALA	2.5
1	A	369	GLY	2.4
1	A	392	GLY	2.4
1	A	156	GLN	2.4
1	A	141	ASP	2.3
1	A	364	PHE	2.3
1	A	359	MET	2.3
1	A	372	GLN	2.3
1	A	253	ILE	2.3
1	A	222	PRO	2.2
1	A	391	ASP	2.2
1	A	315	LYS	2.2
1	A	355	GLY	2.2
1	A	314	GLU	2.1
1	A	194	ARG	2.1
1	A	376	LEU	2.1
1	A	219	ASP	2.1
1	A	225	VAL	2.1
1	A	377	LEU	2.0
1	A	190	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.