



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:49 PM UTC

PDB ID : 3HJ6 / pdb_00003hj6
Title : Structure of Halothermothrix orenii fructokinase (FRK)
Authors : Chua, T.K.; Seetharaman, J.; Kasprzak, J.M.; Ng, C.; Patel, B.K.; Love, C.;
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Deposited on : 2009-05-21
Resolution : 2.80 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

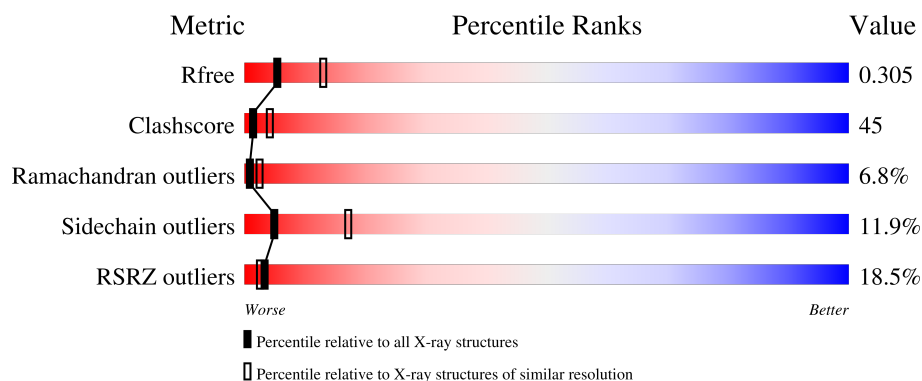
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	327	14% 43% 31% 8% • 15%
1	B	327	17% 39% 36% 7% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4079 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 Fructokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	Se	0	0	0
			1968	1242	341	380	3	2			
1	B	278	Total	C	N	O	S	Se	0	0	0
			1969	1243	341	380	3	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	SEE REMARK 999	UNP B8CZ52
A	2	LYS	-	SEE REMARK 999	UNP B8CZ52
A	3	GLY	-	SEE REMARK 999	UNP B8CZ52
A	4	GLU	-	SEE REMARK 999	UNP B8CZ52
A	5	GLY	-	SEE REMARK 999	UNP B8CZ52
A	6	VAL	-	SEE REMARK 999	UNP B8CZ52
A	7	ILE	-	SEE REMARK 999	UNP B8CZ52
A	8	VAL	-	SEE REMARK 999	UNP B8CZ52
B	1	MSE	-	SEE REMARK 999	UNP B8CZ52
B	2	LYS	-	SEE REMARK 999	UNP B8CZ52
B	3	GLY	-	SEE REMARK 999	UNP B8CZ52
B	4	GLU	-	SEE REMARK 999	UNP B8CZ52
B	5	GLY	-	SEE REMARK 999	UNP B8CZ52
B	6	VAL	-	SEE REMARK 999	UNP B8CZ52
B	7	ILE	-	SEE REMARK 999	UNP B8CZ52
B	8	VAL	-	SEE REMARK 999	UNP B8CZ52

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	86	Total	O	0	0
			86	86		

E287	G288	Y289	T290	V291	K292	R293	S294	I295	K296	L297	G298	K299	G300	V301	A302	A303	F304	K305	I306	ARG	GLY	VAL	GLY	ALA	LEU	SER	PRO	VAL	PRO	SER	LYS	GLU	ASP	ILE	ILE	LYS	GLU	TYR	ASN	ILE
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.45Å 171.94Å 46.60Å 90.00° 112.97° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.5 (50.00-2.80) 95.6 (50.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.288 (Not available) , 0.305	Depositor DCC
R_{free} test set	2069 reflections (6.80%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4079	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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	0.56	0/1999	1.17	22/2708 (0.8%)
1	B	0.57	0/2000	1.19	21/2710 (0.8%)
All	All	0.57	0/3999	1.18	43/5418 (0.8%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	N-CA-C	-13.32	93.17	113.02
1	B	137	ILE	N-CA-C	-10.56	102.37	112.83
1	A	137	ILE	N-CA-C	-10.18	102.76	112.83
1	A	232	TYR	N-CA-C	-9.89	100.35	111.82
1	B	232	TYR	N-CA-C	-9.83	100.54	112.54
1	B	260	ILE	CA-C-N	-9.47	108.58	120.23
1	B	260	ILE	C-N-CA	-9.47	108.58	120.23
1	A	121	ASP	N-CA-C	-9.39	90.81	110.80
1	A	260	ILE	CA-C-N	-9.16	108.96	120.23
1	A	260	ILE	C-N-CA	-9.16	108.96	120.23
1	A	303	ALA	N-CA-C	8.65	129.24	110.80
1	B	291	VAL	N-CA-C	-8.65	101.75	113.00
1	A	302	ALA	N-CA-C	-8.53	97.38	111.37
1	A	291	VAL	N-CA-C	-8.04	102.56	113.00
1	A	158	LYS	N-CA-C	7.01	125.30	109.81
1	B	158	LYS	N-CA-C	6.91	125.09	109.81
1	B	67	LEU	N-CA-C	-6.86	104.79	113.02
1	B	302	ALA	N-CA-C	-6.79	96.33	110.80
1	B	305	LYS	N-CA-C	6.74	119.93	108.67
1	B	233	LEU	N-CA-C	-6.56	105.09	113.23
1	B	30	ILE	N-CA-C	-6.20	99.11	108.17
1	A	30	ILE	N-CA-C	-6.16	99.17	108.17
1	A	67	LEU	N-CA-C	-6.14	105.84	113.15
1	A	304	PHE	N-CA-C	5.96	123.49	110.80
1	A	157	ARG	N-CA-C	5.95	118.65	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	ARG	N-CA-C	5.89	118.56	109.07
1	A	212	SER	N-CA-C	-5.85	101.54	110.14
1	B	212	SER	N-CA-C	-5.82	101.58	110.14
1	A	43	LEU	N-CA-C	-5.79	105.71	112.89
1	A	233	LEU	N-CA-C	-5.66	106.21	113.23
1	B	43	LEU	N-CA-C	-5.62	105.92	112.89
1	B	210	LYS	CA-C-N	-5.49	114.60	120.03
1	B	210	LYS	C-N-CA	-5.49	114.60	120.03
1	A	253	ASP	N-CA-C	-5.46	105.84	112.88
1	B	253	ASP	N-CA-C	-5.23	106.14	112.88
1	B	304	PHE	N-CA-C	-5.22	100.58	108.46
1	A	119	THR	CA-C-N	-5.22	113.32	119.84
1	A	119	THR	C-N-CA	-5.22	113.32	119.84
1	A	292	LYS	N-CA-C	-5.21	106.03	112.38
1	B	285	LEU	N-CA-C	-5.08	107.08	113.28
1	A	227	ASN	N-CA-C	-5.01	107.00	113.01
1	B	116	SER	N-CA-C	5.01	121.47	110.80
1	A	285	LEU	N-CA-C	-5.01	107.17	113.28

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	1968	0	1800	164	0
1	B	1969	0	1801	179	0
2	A	56	0	0	6	0
2	B	86	0	0	16	0
All	All	4079	0	3601	336	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 45.

All (336) 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:260:ILE:HG23	1:B:261:PRO:HD2	1.33	1.10
1:B:260:ILE:HG23	1:B:261:PRO:CD	1.83	1.07
1:A:260:ILE:HG23	1:A:261:PRO:CD	1.83	1.06
1:A:260:ILE:HG23	1:A:261:PRO:HD2	1.40	1.03
1:B:136:ASP:HA	2:B:341:HOH:O	1.62	1.00
1:A:259:ARG:HH11	1:A:259:ARG:HB3	1.30	0.96
1:B:259:ARG:HH11	1:B:259:ARG:HB3	1.31	0.94
1:A:249:VAL:HG12	1:A:260:ILE:CG2	2.01	0.91
1:A:259:ARG:HB3	1:A:259:ARG:NH1	1.86	0.91
1:B:130:MSE:O	1:B:159:PRO:HG2	1.73	0.88
1:B:259:ARG:HB3	1:B:259:ARG:NH1	1.88	0.88
1:A:130:MSE:O	1:A:159:PRO:HG2	1.75	0.86
1:B:249:VAL:HG12	1:B:260:ILE:CG2	2.05	0.85
1:A:291:VAL:HA	2:A:352:HOH:O	1.76	0.84
1:B:137:ILE:HG22	1:B:170:TYR:CD2	2.14	0.83
1:A:301:VAL:HG23	1:A:301:VAL:O	1.81	0.81
1:A:249:VAL:HG12	1:A:260:ILE:HG21	1.62	0.80
1:A:137:ILE:HG22	1:A:170:TYR:CD2	2.17	0.80
1:B:249:VAL:HG12	1:B:260:ILE:HG21	1.63	0.79
1:A:132:LEU:O	1:A:163:THR:HG21	1.82	0.79
1:B:143:LYS:C	1:B:146:LYS:HA	2.09	0.78
1:B:132:LEU:O	1:B:163:THR:HG21	1.83	0.77
1:A:143:LYS:C	1:A:146:LYS:HA	2.10	0.77
1:A:124:PRO:O	1:B:107:ARG:NH1	2.18	0.76
1:A:119:THR:O	1:A:120:PRO:O	2.04	0.76
1:B:77:LEU:HG	1:B:100:ILE:HD11	1.68	0.74
1:A:137:ILE:N	1:A:137:ILE:HD12	2.03	0.74
1:B:122:TRP:CZ3	1:B:124:PRO:HG3	2.23	0.74
1:A:233:LEU:C	1:A:235:LEU:H	1.94	0.73
1:A:235:LEU:O	1:A:237:VAL:N	2.22	0.73
1:A:260:ILE:HG23	1:A:261:PRO:HD3	1.71	0.73
1:B:233:LEU:C	1:B:235:LEU:H	1.96	0.73
1:A:100:ILE:HD13	1:A:101:GLN:N	2.04	0.73
1:B:235:LEU:O	1:B:237:VAL:N	2.22	0.72
1:A:32:VAL:CG2	1:A:110:ILE:HG12	2.19	0.72
1:B:231:ARG:C	1:B:234:GLU:H	1.97	0.72
1:B:100:ILE:HD13	1:B:101:GLN:N	2.05	0.71
1:A:77:LEU:HG	1:A:100:ILE:HD11	1.71	0.71
1:A:283:CYS:C	1:A:285:LEU:H	1.99	0.71
1:B:137:ILE:HD12	1:B:137:ILE:N	2.07	0.70
1:A:222:PRO:O	1:A:224:SER:N	2.24	0.70
1:A:241:ILE:HG12	1:A:249:VAL:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:H	1:A:260:ILE:CG2	2.04	0.69
1:B:222:PRO:O	1:B:224:SER:N	2.25	0.69
1:A:149:HIS:CD2	1:A:278:TRP:HE1	2.11	0.69
1:A:231:ARG:C	1:A:234:GLU:H	2.01	0.69
1:B:32:VAL:CG2	1:B:110:ILE:HG12	2.23	0.69
1:B:114:SER:C	1:B:116:SER:H	2.00	0.69
1:B:283:CYS:C	1:B:285:LEU:H	1.99	0.68
1:B:285:LEU:HA	2:B:349:HOH:O	1.93	0.68
1:A:301:VAL:O	1:A:302:ALA:C	2.37	0.68
1:A:249:VAL:HG12	1:A:260:ILE:HG22	1.75	0.68
1:A:23:ASP:HB2	1:A:70:LYS:O	1.93	0.68
1:B:225:PRO:HD2	1:B:227:ASN:CG	2.18	0.68
1:A:241:ILE:HD13	1:A:241:ILE:O	1.94	0.68
1:A:244:LEU:HD11	1:A:250:ILE:CG1	2.24	0.68
1:A:225:PRO:O	1:A:226:GLU:HG3	1.94	0.67
1:B:241:ILE:HG12	1:B:249:VAL:HG21	1.76	0.67
1:B:97:THR:O	1:B:100:ILE:HG22	1.95	0.67
1:B:149:HIS:CD2	1:B:278:TRP:HE1	2.12	0.67
1:A:225:PRO:HD2	1:A:227:ASN:CG	2.20	0.67
1:A:122:TRP:CZ3	1:A:124:PRO:HG3	2.30	0.66
1:B:23:ASP:HB2	1:B:70:LYS:O	1.95	0.66
1:B:225:PRO:HD2	1:B:227:ASN:ND2	2.10	0.66
1:A:109:THR:HG23	1:A:126:ARG:HA	1.77	0.66
1:B:285:LEU:HD12	1:B:285:LEU:C	2.21	0.65
1:A:225:PRO:HD2	1:A:227:ASN:ND2	2.11	0.65
1:B:225:PRO:HD2	1:B:227:ASN:OD1	1.96	0.65
1:B:249:VAL:H	1:B:260:ILE:CG2	2.09	0.65
1:A:301:VAL:O	1:A:301:VAL:CG2	2.44	0.65
1:B:225:PRO:O	1:B:226:GLU:HG3	1.96	0.65
1:A:77:LEU:HD12	1:A:77:LEU:O	1.97	0.65
1:B:260:ILE:HG12	1:B:297:LEU:HD22	1.78	0.64
1:B:36:SER:O	1:B:114:SER:O	2.16	0.64
1:B:249:VAL:HG12	1:B:260:ILE:HG22	1.80	0.64
1:B:244:LEU:HD11	1:B:250:ILE:CG1	2.28	0.64
1:B:241:ILE:HD13	1:B:241:ILE:O	1.97	0.63
1:B:65:SER:CA	2:B:333:HOH:O	2.45	0.63
1:B:260:ILE:HG23	1:B:261:PRO:HD3	1.79	0.63
1:B:289:TYR:C	1:B:291:VAL:H	2.06	0.63
1:B:290:THR:HG22	1:B:290:THR:O	1.99	0.63
1:B:109:THR:HG23	1:B:126:ARG:HA	1.79	0.63
1:B:32:VAL:HG22	1:B:110:ILE:HG12	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:CZ	1:B:172:ARG:HD2	2.34	0.62
1:A:32:VAL:HG22	1:A:110:ILE:HG12	1.80	0.62
1:A:260:ILE:HG12	1:A:297:LEU:HD22	1.80	0.62
1:A:97:THR:O	1:A:100:ILE:HG22	1.99	0.62
1:A:225:PRO:HD2	1:A:227:ASN:OD1	1.98	0.62
1:B:199:VAL:O	1:B:203:ILE:HG13	2.00	0.62
1:A:44:SER:HB3	1:B:81:ALA:O	2.00	0.61
1:A:290:THR:O	1:A:290:THR:HG22	1.99	0.61
1:A:147:VAL:HG11	1:A:282:ILE:HD12	1.82	0.61
1:A:122:TRP:CE3	1:A:124:PRO:HG3	2.35	0.61
1:A:289:TYR:C	1:A:291:VAL:H	2.07	0.61
1:B:227:ASN:HA	2:B:406:HOH:O	2.00	0.60
1:A:290:THR:C	1:A:292:LYS:H	2.07	0.60
1:A:168:PHE:CZ	1:A:172:ARG:HD2	2.36	0.60
1:B:122:TRP:CE3	1:B:124:PRO:HG3	2.35	0.60
1:B:147:VAL:HG11	1:B:282:ILE:HD12	1.82	0.60
1:A:36:SER:O	1:A:114:SER:O	2.20	0.60
1:B:130:MSE:CE	1:B:157:ARG:HG2	2.31	0.60
1:B:212:SER:H	1:B:215:ASP:HB2	1.66	0.60
1:A:285:LEU:C	1:A:285:LEU:HD12	2.27	0.60
1:A:137:ILE:HD12	1:A:137:ILE:H	1.65	0.59
1:A:199:VAL:O	1:A:203:ILE:HG13	2.02	0.59
1:A:213:LEU:O	1:A:217:ARG:HG3	2.01	0.59
1:A:149:HIS:HD2	1:A:278:TRP:HE1	1.48	0.59
1:A:259:ARG:HH11	1:A:259:ARG:CB	2.10	0.59
1:A:212:SER:H	1:A:215:ASP:HB2	1.67	0.59
1:A:130:MSE:CE	1:A:157:ARG:HG2	2.33	0.58
1:B:290:THR:C	1:B:292:LYS:H	2.09	0.58
1:B:290:THR:C	1:B:292:LYS:N	2.61	0.58
1:B:114:SER:O	1:B:115:LYS:CB	2.50	0.58
1:A:138:ILE:O	1:A:142:ILE:HG12	2.03	0.58
1:B:149:HIS:HD2	1:B:278:TRP:HE1	1.50	0.58
1:B:259:ARG:HH11	1:B:259:ARG:CB	2.12	0.58
1:A:233:LEU:C	1:A:235:LEU:N	2.62	0.58
1:A:260:ILE:CG2	1:A:261:PRO:CD	2.73	0.58
1:A:203:ILE:HG22	1:A:236:GLY:HA2	1.85	0.57
1:B:237:VAL:O	1:B:238:LYS:C	2.47	0.57
1:B:260:ILE:CG2	1:B:261:PRO:CD	2.72	0.57
1:B:260:ILE:HG13	1:B:261:PRO:N	2.20	0.57
1:B:30:ILE:HG22	1:B:75:SER:HB3	1.86	0.56
1:A:237:VAL:O	1:A:238:LYS:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:O	1:B:142:ILE:HG12	2.04	0.56
1:B:255:GLU:HA	2:B:400:HOH:O	2.05	0.56
1:B:291:VAL:HA	2:B:331:HOH:O	2.06	0.56
1:B:137:ILE:HD12	1:B:137:ILE:H	1.69	0.56
1:B:301:VAL:C	1:B:302:ALA:O	2.44	0.56
1:B:77:LEU:HD12	1:B:77:LEU:O	2.06	0.55
1:B:203:ILE:HG22	1:B:236:GLY:HA2	1.87	0.55
1:A:119:THR:C	1:A:120:PRO:O	2.49	0.55
1:B:137:ILE:HG22	1:B:170:TYR:CE2	2.41	0.55
1:B:213:LEU:O	1:B:217:ARG:HG3	2.07	0.55
1:B:106:ARG:HG3	1:B:106:ARG:HH11	1.70	0.54
1:A:27:LEU:C	1:A:27:LEU:HD23	2.32	0.54
1:B:291:VAL:CA	2:B:331:HOH:O	2.55	0.54
1:A:290:THR:C	1:A:292:LYS:N	2.61	0.54
1:B:35:ILE:CD1	1:B:113:VAL:HB	2.38	0.54
1:A:35:ILE:CD1	1:A:113:VAL:HB	2.38	0.54
1:B:234:GLU:C	1:B:236:GLY:H	2.14	0.54
1:A:60:ILE:HD12	1:A:149:HIS:CE1	2.44	0.53
1:A:44:SER:HB2	1:B:85:TYR:HB2	1.89	0.53
1:A:234:GLU:C	1:A:236:GLY:H	2.17	0.53
1:A:280:GLY:HA3	1:A:296:LYS:HA	1.91	0.53
1:B:130:MSE:SE	1:B:157:ARG:HG2	2.59	0.53
1:A:106:ARG:HG3	1:A:106:ARG:HH11	1.73	0.52
1:A:249:VAL:H	1:A:260:ILE:HG22	1.75	0.52
1:B:260:ILE:HG12	1:B:297:LEU:CD2	2.39	0.52
1:B:241:ILE:CG1	1:B:249:VAL:HG21	2.40	0.52
1:B:280:GLY:HA3	1:B:296:LYS:HA	1.92	0.52
1:A:184:TYR:HB2	1:A:199:VAL:HG21	1.92	0.52
1:A:213:LEU:HB2	2:A:342:HOH:O	2.10	0.51
1:B:146:LYS:N	2:B:368:HOH:O	2.41	0.51
1:A:204:SER:O	1:A:237:VAL:HG22	2.10	0.51
1:B:60:ILE:HD12	1:B:149:HIS:CE1	2.46	0.51
1:B:113:VAL:HG12	1:B:114:SER:N	2.25	0.51
1:A:241:ILE:CG1	1:A:249:VAL:HG21	2.40	0.51
1:B:64:LEU:HB2	1:B:71:VAL:HG21	1.92	0.51
1:A:130:MSE:SE	1:A:157:ARG:HG2	2.61	0.51
1:B:225:PRO:HD2	1:B:227:ASN:HD21	1.76	0.51
1:B:229:VAL:HG12	1:B:229:VAL:O	2.10	0.50
1:B:233:LEU:C	1:B:235:LEU:N	2.63	0.50
1:A:289:TYR:C	1:A:291:VAL:N	2.70	0.49
1:A:46:SER:HB2	1:A:49:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HD11	1:A:250:ILE:HG13	1.94	0.49
1:A:260:ILE:HG13	1:A:261:PRO:N	2.25	0.49
1:A:225:PRO:HD2	1:A:227:ASN:HD21	1.77	0.49
1:B:289:TYR:C	1:B:291:VAL:N	2.70	0.49
1:A:28:GLY:HA3	1:A:57:PRO:HG2	1.94	0.49
1:A:137:ILE:N	1:A:137:ILE:CD1	2.73	0.49
1:A:134:GLU:HG3	1:A:163:THR:HB	1.93	0.49
1:A:137:ILE:HG22	1:A:170:TYR:CE2	2.48	0.49
1:A:229:VAL:HG12	1:A:229:VAL:O	2.12	0.49
1:B:28:GLY:HA3	1:B:57:PRO:HG2	1.94	0.49
1:A:30:ILE:HG22	1:A:75:SER:HB3	1.95	0.49
1:B:150:LEU:HD22	1:B:151:SER:N	2.28	0.49
1:B:297:LEU:HD23	2:B:380:HOH:O	2.13	0.48
1:A:64:LEU:HB2	1:A:71:VAL:HG21	1.95	0.48
1:B:22:LEU:N	2:B:355:HOH:O	2.46	0.48
1:B:46:SER:HB2	1:B:49:TYR:OH	2.13	0.48
1:A:77:LEU:HD12	1:A:77:LEU:C	2.39	0.48
1:A:101:GLN:NE2	1:A:132:LEU:HD12	2.28	0.48
1:B:137:ILE:N	1:B:137:ILE:CD1	2.77	0.48
1:A:35:ILE:HD12	1:A:113:VAL:HB	1.96	0.48
1:B:143:LYS:O	1:B:146:LYS:HA	2.13	0.48
1:B:184:TYR:HB2	1:B:199:VAL:HG21	1.95	0.48
1:B:157:ARG:HD2	1:B:158:LYS:HE2	1.96	0.48
1:A:76:ARG:HG2	1:A:128:ALA:HB1	1.96	0.48
1:B:210:LYS:NZ	1:B:210:LYS:HB3	2.28	0.47
1:B:76:ARG:HG2	1:B:128:ALA:HB1	1.97	0.47
1:B:114:SER:C	1:B:116:SER:N	2.68	0.47
1:B:134:GLU:HG3	1:B:163:THR:HB	1.96	0.47
1:A:80:ASP:OD1	1:A:107:ARG:HD3	2.15	0.47
1:B:106:ARG:HG3	1:B:106:ARG:NH1	2.28	0.47
1:B:155:LEU:O	1:B:161:ARG:HB2	2.14	0.47
1:B:256:GLU:OE2	1:B:258:ILE:HD11	2.14	0.47
1:A:112:TYR:CE2	1:B:34:MSE:HE3	2.50	0.47
1:A:210:LYS:HD2	1:A:210:LYS:O	2.15	0.47
1:B:27:LEU:HD23	1:B:27:LEU:C	2.40	0.47
1:B:150:LEU:HD22	1:B:151:SER:H	1.78	0.47
1:A:283:CYS:O	1:A:285:LEU:N	2.48	0.47
1:B:204:SER:HA	1:B:235:LEU:C	2.40	0.47
1:A:76:ARG:HH21	1:A:133:GLN:HG2	1.80	0.46
1:A:155:LEU:O	1:A:161:ARG:HB2	2.14	0.46
1:A:260:ILE:HG12	1:A:297:LEU:CD2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:HG2	1:B:259:ARG:NH2	2.29	0.46
1:A:106:ARG:HG3	1:A:106:ARG:NH1	2.30	0.46
1:A:47:ARG:O	1:B:50:THR:HA	2.16	0.46
1:B:258:ILE:HD12	1:B:258:ILE:N	2.31	0.46
1:B:249:VAL:H	1:B:260:ILE:HG22	1.81	0.46
1:A:123:LEU:HD22	1:B:107:ARG:HD2	1.97	0.46
1:A:225:PRO:C	1:A:226:GLU:HG3	2.40	0.46
1:A:249:VAL:O	1:A:260:ILE:HG22	2.16	0.46
1:A:112:TYR:O	1:A:122:TRP:HA	2.16	0.46
1:A:206:ALA:O	1:A:237:VAL:HG23	2.16	0.46
1:B:217:ARG:HG2	1:B:217:ARG:HH11	1.80	0.46
1:A:30:ILE:O	1:A:30:ILE:HG23	2.16	0.46
1:A:149:HIS:CD2	1:A:278:TRP:NE1	2.82	0.46
1:A:210:LYS:NZ	1:A:210:LYS:HB3	2.31	0.46
1:A:250:ILE:HA	1:A:258:ILE:O	2.16	0.46
1:B:51:ARG:HD2	1:B:51:ARG:C	2.40	0.46
1:B:250:ILE:HA	1:B:258:ILE:O	2.15	0.46
1:A:140:GLU:N	1:A:140:GLU:OE2	2.49	0.45
1:A:154:ILE:HD11	1:A:160:ALA:HB1	1.98	0.45
1:A:150:LEU:HD22	1:A:151:SER:N	2.31	0.45
1:A:243:THR:HA	1:A:249:VAL:HG23	1.98	0.45
1:B:143:LYS:CB	2:B:375:HOH:O	2.64	0.45
1:B:204:SER:O	1:B:237:VAL:HG22	2.16	0.45
1:B:233:LEU:O	1:B:235:LEU:N	2.49	0.45
1:B:257:ILE:C	1:B:258:ILE:HD12	2.42	0.45
1:A:100:ILE:HD13	1:A:100:ILE:C	2.42	0.45
1:B:149:HIS:CD2	1:B:278:TRP:NE1	2.83	0.45
1:B:249:VAL:O	1:B:260:ILE:HG22	2.16	0.45
1:B:288:GLY:O	1:B:289:TYR:O	2.34	0.45
1:A:160:ALA:O	1:A:163:THR:HG23	2.17	0.45
1:A:247:GLU:HG2	1:A:259:ARG:NH2	2.32	0.45
1:A:258:ILE:N	1:A:258:ILE:HD12	2.32	0.45
1:B:140:GLU:OE2	1:B:140:GLU:N	2.50	0.45
1:A:288:GLY:O	1:A:289:TYR:O	2.35	0.45
1:B:130:MSE:HE1	1:B:157:ARG:NH1	2.32	0.45
1:A:304:PHE:O	1:A:305:LYS:C	2.58	0.45
1:B:283:CYS:C	1:B:285:LEU:N	2.67	0.45
1:A:157:ARG:HD2	1:A:158:LYS:HE2	1.99	0.44
1:A:287:ASP:OD2	1:A:288:GLY:N	2.50	0.44
1:B:101:GLN:NE2	1:B:132:LEU:HD12	2.32	0.44
1:A:209:VAL:CG2	1:A:240:VAL:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:CG2	1:B:75:SER:HB3	2.46	0.44
1:B:235:LEU:O	1:B:237:VAL:HG22	2.18	0.44
1:B:283:CYS:O	1:B:285:LEU:N	2.49	0.44
1:A:130:MSE:C	1:A:160:ALA:HB2	2.43	0.44
1:A:241:ILE:HG12	1:A:249:VAL:CG2	2.43	0.44
1:B:158:LYS:H	1:B:158:LYS:HG3	1.61	0.44
1:A:60:ILE:HD13	1:A:278:TRP:HD1	1.82	0.44
1:A:233:LEU:O	1:A:235:LEU:N	2.48	0.44
1:B:225:PRO:C	1:B:226:GLU:HG3	2.42	0.44
1:A:256:GLU:OE2	1:A:258:ILE:HD11	2.17	0.44
1:B:100:ILE:HG12	2:B:342:HOH:O	2.16	0.44
1:A:157:ARG:HG3	1:A:158:LYS:HE2	1.99	0.44
1:A:130:MSE:HE1	1:A:157:ARG:NH1	2.33	0.43
1:A:143:LYS:O	1:A:146:LYS:HA	2.17	0.43
1:B:22:LEU:N	2:B:374:HOH:O	2.50	0.43
1:A:209:VAL:HG23	1:A:240:VAL:HG23	2.00	0.43
1:A:36:SER:HB2	1:A:49:TYR:CE1	2.53	0.43
1:A:51:ARG:C	1:A:51:ARG:HD2	2.44	0.43
1:A:228:TYR:C	1:A:230:LYS:H	2.27	0.43
1:A:283:CYS:C	1:A:285:LEU:N	2.67	0.43
1:B:209:VAL:CG2	1:B:240:VAL:HB	2.48	0.43
1:B:228:TYR:C	1:B:230:LYS:H	2.26	0.43
1:B:285:LEU:C	1:B:285:LEU:CD1	2.89	0.43
1:A:204:SER:HA	1:A:235:LEU:C	2.43	0.43
1:A:217:ARG:HH11	1:A:217:ARG:HG2	1.83	0.43
1:A:226:GLU:C	1:A:228:TYR:N	2.77	0.43
1:B:206:ALA:O	1:B:237:VAL:HG23	2.19	0.43
1:A:36:SER:HB2	1:A:49:TYR:CD1	2.54	0.43
1:A:235:LEU:C	1:A:237:VAL:H	2.27	0.43
1:A:290:THR:C	2:A:330:HOH:O	2.62	0.43
1:B:143:LYS:O	1:B:146:LYS:CB	2.66	0.43
1:B:259:ARG:HD2	2:B:369:HOH:O	2.19	0.43
1:B:244:LEU:HD11	1:B:250:ILE:HG13	1.98	0.43
1:A:217:ARG:CZ	2:A:372:HOH:O	2.67	0.43
1:A:257:ILE:C	1:A:258:ILE:HD12	2.44	0.43
1:B:130:MSE:C	1:B:160:ALA:HB2	2.43	0.43
1:B:228:TYR:C	1:B:230:LYS:N	2.77	0.43
1:B:241:ILE:HG12	1:B:249:VAL:CG2	2.46	0.43
1:B:100:ILE:HD13	1:B:100:ILE:C	2.44	0.42
1:B:242:LEU:C	1:B:249:VAL:HG23	2.44	0.42
1:B:35:ILE:HD12	1:B:113:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLY:C	2:B:390:HOH:O	2.62	0.42
1:A:107:ARG:NH1	1:B:124:PRO:O	2.52	0.42
1:A:186:LYS:N	2:A:331:HOH:O	2.53	0.42
1:A:228:TYR:C	1:A:230:LYS:N	2.77	0.42
1:B:30:ILE:O	1:B:30:ILE:HG23	2.19	0.42
1:B:80:ASP:OD1	1:B:107:ARG:HD3	2.19	0.42
1:B:36:SER:HB2	1:B:49:TYR:CE1	2.54	0.42
1:B:71:VAL:HG12	1:B:72:ALA:N	2.35	0.42
1:A:235:LEU:C	1:A:237:VAL:N	2.78	0.42
1:B:56:SER:O	1:B:60:ILE:HG13	2.18	0.42
1:B:64:LEU:CB	1:B:71:VAL:HG21	2.49	0.42
1:B:235:LEU:C	1:B:237:VAL:N	2.78	0.42
1:B:76:ARG:HH21	1:B:133:GLN:HG2	1.83	0.42
1:B:77:LEU:HD12	1:B:77:LEU:C	2.45	0.42
1:B:160:ALA:O	1:B:163:THR:HG23	2.20	0.42
1:A:178:VAL:CG2	1:A:206:ALA:HA	2.49	0.42
1:B:210:LYS:HD2	1:B:210:LYS:O	2.19	0.42
1:B:217:ARG:HG2	1:B:217:ARG:NH1	2.35	0.41
1:B:133:GLN:NE2	2:B:399:HOH:O	2.49	0.41
1:A:150:LEU:HD22	1:A:151:SER:H	1.84	0.41
1:B:30:ILE:HD12	1:B:58:ALA:CB	2.50	0.41
1:B:235:LEU:C	1:B:237:VAL:H	2.28	0.41
1:A:158:LYS:H	1:A:158:LYS:HG3	1.56	0.41
1:B:154:ILE:HD11	1:B:160:ALA:HB1	2.02	0.41
1:B:231:ARG:C	1:B:233:LEU:N	2.76	0.41
1:B:277:PHE:O	1:B:296:LYS:CB	2.69	0.41
1:A:143:LYS:O	1:A:146:LYS:CB	2.68	0.41
1:A:226:GLU:C	1:A:228:TYR:H	2.29	0.41
1:A:30:ILE:CG2	1:A:75:SER:HB3	2.51	0.41
1:B:247:GLU:HG2	1:B:259:ARG:HH22	1.86	0.41
1:A:64:LEU:CB	1:A:71:VAL:HG21	2.51	0.41
1:A:235:LEU:O	1:A:237:VAL:HG22	2.20	0.41
1:A:244:LEU:HD11	1:A:250:ILE:HD11	2.02	0.41
1:B:165:ILE:HA	1:B:168:PHE:HB3	2.03	0.41
1:B:209:VAL:HG23	1:B:240:VAL:HG23	2.03	0.41
1:A:285:LEU:C	1:A:285:LEU:CD1	2.94	0.40
1:A:301:VAL:O	1:A:302:ALA:O	2.38	0.40
1:B:178:VAL:CG2	1:B:206:ALA:HA	2.51	0.40
1:B:189:TRP:HA	1:B:190:PRO:HD3	1.88	0.40
1:A:113:VAL:HG12	1:A:114:SER:N	2.36	0.40
1:A:272:GLY:N	2:A:333:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:HA	1:B:249:VAL:HG23	2.01	0.40
1:B:35:ILE:HD13	1:B:113:VAL:HB	2.03	0.40
1:B:137:ILE:CG2	1:B:170:TYR:CD2	2.97	0.40
1:B:198:VAL:O	1:B:202:ILE:HG13	2.22	0.40
1:B:210:LYS:HA	1:B:241:ILE:HD13	2.03	0.40
1:B:157:ARG:HG3	1:B:158:LYS:HE2	2.04	0.40
1:B:226:GLU:C	1:B:228:TYR:N	2.79	0.40

There are no symmetry-related clashes.

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	272/327 (83%)	228 (84%)	24 (9%)	20 (7%)	1	2
1	B	272/327 (83%)	232 (85%)	23 (8%)	17 (6%)	1	3
All	All	544/654 (83%)	460 (85%)	47 (9%)	37 (7%)	1	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	120	PRO
1	A	121	ASP
1	A	223	ASP
1	A	224	SER
1	A	236	GLY
1	A	303	ALA
1	A	304	PHE
1	B	116	SER
1	B	117	THR
1	B	223	ASP

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Mol	Chain	Res	Type
1	B	224	SER
1	B	236	GLY
1	B	260	ILE
1	A	237	VAL
1	A	260	ILE
1	A	289	TYR
1	A	305	LYS
1	B	237	VAL
1	B	289	TYR
1	A	115	LYS
1	B	302	ALA
1	A	127	GLU
1	A	234	GLU
1	B	127	GLU
1	B	234	GLU
1	A	226	GLU
1	B	121	ASP
1	B	226	GLU
1	A	158	LYS
1	B	158	LYS
1	B	159	PRO
1	A	159	PRO
1	B	225	PRO
1	B	229	VAL
1	A	225	PRO
1	A	229	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	185/272 (68%)	165 (89%)	20 (11%)	6	21
1	B	185/272 (68%)	161 (87%)	24 (13%)	4	14
All	All	370/544 (68%)	326 (88%)	44 (12%)	5	17

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	73	LEU
1	A	89	VAL
1	A	100	ILE
1	A	102	GLN
1	A	123	LEU
1	A	127	GLU
1	A	137	ILE
1	A	150	LEU
1	A	157	ARG
1	A	161	ARG
1	A	163	THR
1	A	165	ILE
1	A	188	LEU
1	A	210	LYS
1	A	227	ASN
1	A	237	VAL
1	A	240	VAL
1	A	241	ILE
1	A	295	ILE
1	B	30	ILE
1	B	73	LEU
1	B	89	VAL
1	B	100	ILE
1	B	102	GLN
1	B	114	SER
1	B	123	LEU
1	B	127	GLU
1	B	129	ASP
1	B	137	ILE
1	B	150	LEU
1	B	157	ARG
1	B	161	ARG
1	B	163	THR
1	B	165	ILE
1	B	188	LEU
1	B	210	LYS
1	B	227	ASN
1	B	237	VAL
1	B	240	VAL
1	B	241	ILE
1	B	295	ILE
1	B	299	ASN

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Mol	Chain	Res	Type
1	B	301	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	149	HIS
1	B	52	HIS
1	B	149	HIS
1	B	218	HIS

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	276/327 (84%)	1.18	47 (17%) 4 3	25, 46, 74, 110	0
1	B	276/327 (84%)	1.28	55 (19%) 3 2	25, 45, 70, 88	0
All	All	552/654 (84%)	1.23	102 (18%) 3 2	25, 46, 73, 110	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	ILE	4.9
1	A	237	VAL	4.7
1	A	260	ILE	4.0
1	A	120	PRO	4.0
1	B	239	ALA	3.9
1	B	287	ASP	3.7
1	B	120	PRO	3.6
1	B	291	VAL	3.5
1	B	42	SER	3.4
1	A	302	ALA	3.4
1	B	238	LYS	3.2
1	B	301	VAL	3.1
1	A	286	LEU	3.1
1	B	223	ASP	3.1
1	B	303	ALA	3.0
1	B	237	VAL	3.0
1	B	117	THR	3.0
1	B	306	ILE	3.0
1	B	224	SER	2.9
1	B	293	ARG	2.9
1	A	141	LEU	2.9
1	B	22	LEU	2.9
1	A	236	GLY	2.9
1	B	266	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	137	ILE	2.9
1	B	142	ILE	2.9
1	A	226	GLU	2.9
1	A	301	VAL	2.8
1	A	303	ALA	2.8
1	A	143	LYS	2.8
1	B	236	GLY	2.8
1	A	225	PRO	2.8
1	B	304	PHE	2.8
1	B	41	ASN	2.8
1	B	290	THR	2.8
1	A	42	SER	2.8
1	B	118	ARG	2.7
1	B	285	LEU	2.7
1	B	139	PHE	2.7
1	A	232	TYR	2.7
1	A	266	ASP	2.6
1	A	142	ILE	2.6
1	A	178	VAL	2.6
1	B	289	TYR	2.6
1	A	284	GLY	2.6
1	A	117	THR	2.6
1	A	222	PRO	2.6
1	B	241	ILE	2.6
1	B	40	VAL	2.5
1	B	171	ALA	2.5
1	A	287	ASP	2.5
1	A	291	VAL	2.5
1	A	168	PHE	2.4
1	A	41	ASN	2.4
1	A	137	ILE	2.4
1	B	99	GLY	2.4
1	B	173	GLU	2.4
1	A	44	SER	2.4
1	A	22	LEU	2.4
1	B	158	LYS	2.3
1	B	68	GLY	2.3
1	B	78	GLY	2.3
1	A	300	GLY	2.3
1	A	45	GLN	2.3
1	B	143	LYS	2.3
1	B	305	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	172	ARG	2.3
1	B	38	GLU	2.3
1	B	233	LEU	2.3
1	A	163	THR	2.3
1	A	191	GLU	2.3
1	B	147	VAL	2.3
1	B	226	GLU	2.2
1	B	96	ILE	2.2
1	B	257	ILE	2.2
1	A	217	ARG	2.2
1	A	289	TYR	2.2
1	A	299	ASN	2.2
1	A	223	ASP	2.2
1	A	119	THR	2.2
1	B	252	SER	2.2
1	B	225	PRO	2.2
1	B	112	TYR	2.2
1	B	170	TYR	2.2
1	A	146	LYS	2.1
1	B	259	ARG	2.1
1	B	121	ASP	2.1
1	B	193	ASP	2.1
1	A	122	TRP	2.1
1	A	290	THR	2.1
1	B	163	THR	2.1
1	A	278	TRP	2.1
1	B	246	GLU	2.1
1	A	158	LYS	2.1
1	A	118	ARG	2.1
1	B	213	LEU	2.0
1	B	222	PRO	2.0
1	A	259	ARG	2.0
1	A	202	ILE	2.0
1	A	241	ILE	2.0
1	A	171	ALA	2.0
1	A	206	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.