



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:25 PM UTC

PDB ID : 8SAP / pdb_00008sap
Title : Crystal structure of class III lanthipeptide synthetase ThurKC
Authors : Hernandez Garcia, A.; Nair, S.K.
Deposited on : 2023-04-01
Resolution : 2.52 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

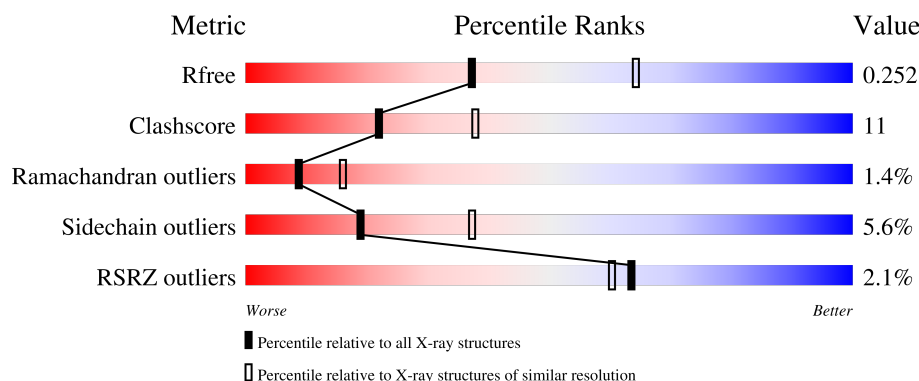
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	875	3% 73% 20% • 5%
1	B	875	% 72% 22% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13906 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 Class III lanthionine synthetase LanKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6723	4322	1109	1270	22			
1	B	842	Total	C	N	O	S	0	0	0
			6799	4368	1123	1285	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A6H0TJ16
A	-1	ASN	-	expression tag	UNP A0A6H0TJ16
A	0	ALA	-	expression tag	UNP A0A6H0TJ16
B	-2	SER	-	expression tag	UNP A0A6H0TJ16
B	-1	ASN	-	expression tag	UNP A0A6H0TJ16
B	0	ALA	-	expression tag	UNP A0A6H0TJ16

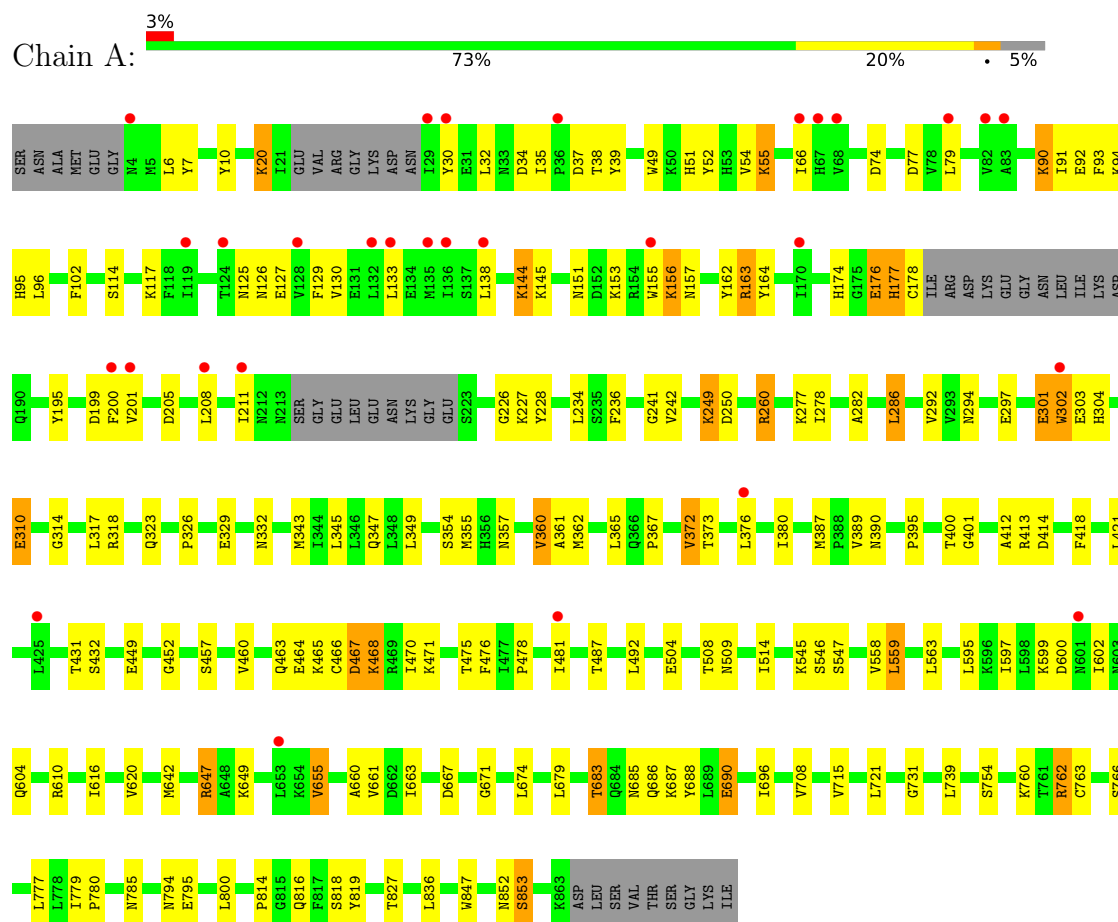
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		
2	B	224	Total	O	0	0
			224	224		

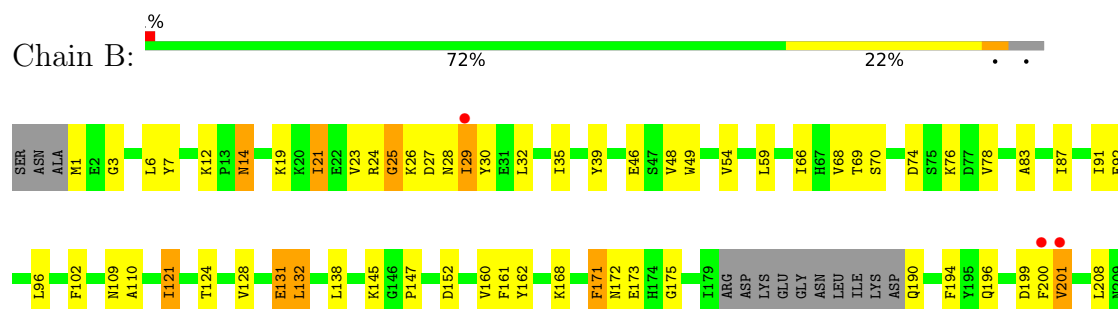
3 Residue-property plots

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: Class III lanthionine synthetase LanKC



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T210	T211	ASN	ASN	SER	GLY	GLU	LEU	GLU	ASN	LYS	GLY	GLU	S223	K227	Y228	S237	Y243	T246	R247	K248	K249	D250	K253	I256	K257	E258	A259	R260	P261	G264	L265	D266	Q270	R275	V292	E297	Q300	E301	W302	E303	F306	I307	V308	R318
F325	M334	I338	M343	Q347	L351	M355	A361	M362	G363	D364	L365	G366	P367	A368	N369	V372	T373	L376	T377	I380	F383	P388	V389	N390	S391	T399	T400	Q401	V409	F418	K419	R420	P428	T431	S432	E436	G437	Y438	F455	Y456				
V460	C466	I481	L492	E504	N509	R512	F513	I514	E522	M523	K527	F530	S546	S547	V558	L559	L563	P564	L565	I566	E567	K575	L579	L595	K599	D600	R601	I602	T605	R610	L613	I616	V620	L625	E626	T627								
E628	M629	E640	R641	M642	T643	R644	L645	M646	R647	D650	L653	R654	V655	M658	R659	M660	V661	D662	I663	D667	S673	L679	V682	T683	Q684	M685	V688	K697	D706	D707	V708	T709	V715	D716	M717	K718	M719	R720	N740	L747	S754	K760		
I765	S766	L777	L778	I779	P780	N785	D786	K787	N788	R789	N794	L800	K807	Q816	F817	S818	Y819	T827	L836	M847	L848	P849	K863	ASP	LEU	SER	VAL	THR	SER	GLY	LYS	ILE												

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.30Å 230.23Å 84.38Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	115.11 – 2.52 115.11 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.9 (115.11-2.52) 98.9 (115.11-2.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.250 0.191 , 0.252	Depositor DCC
R_{free} test set	3422 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.2	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	0.96	EDS
Total number of atoms	13906	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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	0.47	0/6855	1.03	7/9250 (0.1%)
1	B	0.49	0/6932	1.05	4/9351 (0.0%)
All	All	0.48	0/13787	1.04	11/18601 (0.1%)

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	B	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	400	THR	CA-C-N	-5.96	116.34	123.44
1	B	400	THR	C-N-CA	-5.96	116.34	123.44
1	A	785	ASN	CB-CA-C	5.77	119.05	109.53
1	A	508	THR	CA-C-N	-5.75	113.47	122.73
1	A	508	THR	C-N-CA	-5.75	113.47	122.73
1	A	400	THR	CB-CA-C	5.54	118.62	109.70
1	A	278	ILE	N-CA-C	-5.40	107.53	111.90
1	A	509	ASN	CB-CA-C	5.37	119.80	110.94
1	B	258	GLU	CB-CA-C	-5.22	99.93	109.54
1	A	794	ASN	CB-CA-C	5.18	119.66	110.85
1	B	171	PHE	CB-CA-C	5.04	118.45	110.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6723	0	6717	125	0
1	B	6799	0	6807	164	0
2	A	160	0	0	9	0
2	B	224	0	0	21	0
All	All	13906	0	13524	288	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 11.

All (288) 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:647:ARG:HG2	1:A:647:ARG:HH11	1.20	1.03
1:B:605:THR:HA	1:B:646:ASN:HD21	1.27	0.99
1:B:431:THR:HG21	1:B:436:GLU:OE1	1.63	0.96
1:A:286:LEU:CD1	1:A:292:VAL:HG11	1.98	0.93
1:B:28:ASN:O	1:B:30:TYR:N	2.05	0.90
1:B:683:THR:CG2	1:B:685:ASN:HB3	2.04	0.88
1:A:683:THR:CG2	1:A:685:ASN:HB3	2.06	0.84
1:A:471:LYS:HD3	1:A:476:PHE:O	1.76	0.84
1:A:355:MET:HE1	1:A:380:ILE:HD12	1.58	0.83
1:B:70:SER:HB2	1:B:78:VAL:HG11	1.63	0.81
1:B:716:ASP:HB3	1:B:718:LYS:H	1.47	0.79
1:B:605:THR:HA	1:B:646:ASN:ND2	1.98	0.78
1:A:604:GLN:HG2	1:A:642:MET:HE3	1.68	0.76
1:A:647:ARG:HG2	1:A:647:ARG:NH1	1.95	0.75
1:A:226:GLY:HA2	2:A:990:HOH:O	1.86	0.75
1:B:628:GLU:N	2:B:904:HOH:O	2.18	0.74
1:B:760:LYS:HE2	2:B:1025:HOH:O	1.86	0.74
1:B:301:GLU:O	2:B:902:HOH:O	2.05	0.74
1:B:627:THR:O	1:B:627:THR:OG1	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:HD23	1:A:414:ASP:O	1.88	0.73
1:A:387:MET:HE1	1:A:395:PRO:HA	1.69	0.73
1:B:70:SER:CB	1:B:78:VAL:HG11	2.18	0.72
1:A:286:LEU:HD13	1:A:292:VAL:HG21	1.72	0.72
1:B:401:GLY:HA2	1:B:431:THR:O	1.89	0.72
1:B:69:THR:HG22	1:B:70:SER:N	2.05	0.71
1:B:683:THR:HG23	1:B:685:ASN:HB3	1.73	0.70
1:A:286:LEU:HD23	1:A:360:VAL:HG11	1.72	0.70
1:A:487:THR:O	2:A:901:HOH:O	2.10	0.69
1:B:338:ILE:HG23	1:B:455:PHE:CD1	2.28	0.69
1:B:567:GLU:H	1:B:567:GLU:CD	1.97	0.69
1:B:683:THR:HG22	1:B:685:ASN:H	1.58	0.69
1:B:83:ALA:O	1:B:87:ILE:HG12	1.94	0.68
1:A:286:LEU:HD12	1:A:292:VAL:HG11	1.75	0.68
1:A:286:LEU:HD13	1:A:292:VAL:HG11	1.72	0.68
1:A:683:THR:HG23	1:A:685:ASN:HB3	1.73	0.67
1:B:3:GLY:O	1:B:6:LEU:HB2	1.93	0.67
1:A:114:SER:HA	1:A:117:LYS:HE2	1.74	0.67
1:A:421:LEU:HD23	1:A:421:LEU:O	1.95	0.67
1:B:74:ASP:O	1:B:78:VAL:HG12	1.94	0.67
1:B:627:THR:C	2:B:904:HOH:O	2.36	0.67
1:B:456:TYR:CZ	1:B:460:VAL:HG21	2.30	0.67
1:A:176:GLU:O	1:A:177:HIS:HB2	1.94	0.67
1:A:457:SER:HA	1:A:460:VAL:HG12	1.76	0.67
1:A:545:LYS:NZ	1:B:794:ASN:OD1	2.28	0.66
1:A:163:ARG:HD3	1:A:164:TYR:H	1.60	0.66
1:A:7:TYR:OH	1:A:816:GLN:HG3	1.97	0.65
1:A:401:GLY:HA2	1:A:431:THR:O	1.96	0.65
1:A:683:THR:HG22	1:A:685:ASN:H	1.61	0.65
1:B:504:GLU:HG2	1:B:547:SER:OG	1.97	0.65
1:A:655:VAL:HG13	1:A:660:ALA:HB3	1.78	0.64
1:B:355:MET:HE3	1:B:380:ILE:HD13	1.79	0.64
1:A:465:LYS:O	2:A:902:HOH:O	2.15	0.63
1:A:683:THR:HG21	1:A:688:TYR:CD2	2.34	0.63
1:A:282:ALA:O	1:A:286:LEU:HG	1.98	0.63
1:B:7:TYR:OH	1:B:816:GLN:HG3	1.97	0.63
1:B:28:ASN:C	1:B:30:TYR:H	2.00	0.63
1:B:12:LYS:HA	1:B:21:ILE:HG22	1.81	0.63
1:B:373:THR:HG22	1:B:377:THR:H	1.64	0.63
1:B:12:LYS:HA	1:B:21:ILE:CG2	2.29	0.62
1:B:69:THR:HG22	1:B:70:SER:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:MET:HE2	1:B:658:TRP:CZ3	2.34	0.62
1:B:683:THR:HG21	1:B:688:TYR:CD2	2.35	0.61
1:A:604:GLN:CG	1:A:642:MET:HE3	2.29	0.61
1:A:679:LEU:O	1:A:683:THR:HB	2.01	0.60
1:A:286:LEU:HD23	1:A:360:VAL:CG1	2.29	0.60
1:A:602:ILE:CG2	1:A:642:MET:HE1	2.31	0.60
1:A:687:LYS:NZ	2:A:907:HOH:O	2.35	0.60
1:A:176:GLU:OE1	1:A:178:CYS:HB3	2.01	0.59
1:A:301:GLU:O	1:A:302:TRP:C	2.45	0.59
1:B:343:MET:HG2	1:B:347:GLN:HE21	1.67	0.59
1:A:413:ARG:HD3	2:A:1031:HOH:O	2.02	0.59
1:B:243:TYR:HE2	1:B:258:GLU:HG3	1.66	0.59
1:B:1:MET:HG3	1:B:3:GLY:H	1.68	0.59
1:B:91:ILE:HG13	1:B:132:LEU:HD21	1.84	0.59
1:B:351:LEU:HD21	1:B:380:ILE:HD12	1.85	0.59
1:B:786:ASP:OD1	1:B:789:ARG:NH1	2.35	0.58
1:B:679:LEU:O	1:B:683:THR:HB	2.02	0.58
1:B:301:GLU:O	1:B:302:TRP:C	2.45	0.58
1:B:171:PHE:HB3	1:B:175:GLY:HA2	1.85	0.58
1:A:130:VAL:HG12	1:A:208:LEU:HD21	1.85	0.58
1:A:354:SER:O	1:A:357:ASN:HB2	2.03	0.58
1:B:785:ASN:OD1	1:B:788:ASN:HB2	2.04	0.58
1:A:343:MET:HG2	1:A:347:GLN:HE21	1.70	0.56
1:A:602:ILE:HG23	1:A:642:MET:HE1	1.87	0.56
1:B:69:THR:CG2	1:B:70:SER:H	2.19	0.56
1:B:655:VAL:HG13	1:B:660:ALA:HB3	1.88	0.56
1:B:162:TYR:O	2:B:903:HOH:O	2.17	0.55
1:B:69:THR:CG2	1:B:70:SER:N	2.69	0.55
1:B:303:GLU:HB3	2:B:921:HOH:O	2.05	0.55
1:B:355:MET:CE	1:B:380:ILE:HD13	2.36	0.55
1:B:523:MET:HE2	1:B:658:TRP:HZ3	1.72	0.55
1:A:294:ASN:H	1:A:310:GLU:HG2	1.72	0.55
1:B:388:PRO:O	1:B:391:SER:HB3	2.06	0.54
1:A:610:ARG:HD2	1:A:667:ASP:OD2	2.07	0.54
1:A:816:GLN:HG2	1:A:827:THR:HG21	1.89	0.54
1:B:627:THR:C	1:B:629:ASN:H	2.14	0.54
1:B:246:THR:HG22	1:B:253:LYS:HD2	1.90	0.54
1:B:69:THR:HG23	2:B:1038:HOH:O	2.07	0.54
1:B:683:THR:HG21	1:B:688:TYR:CE2	2.42	0.54
1:B:740:ASN:HD21	1:B:747:LEU:H	1.55	0.54
1:B:373:THR:HG22	1:B:377:THR:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE2	1:B:658:TRP:HB2	1.89	0.54
1:A:683:THR:HG23	1:A:685:ASN:CB	2.37	0.54
1:B:334:MET:O	1:B:338:ILE:HG13	2.08	0.54
1:B:318:ARG:HG2	1:B:367:PRO:HB2	1.91	0.53
1:B:627:THR:O	1:B:629:ASN:N	2.39	0.53
1:A:558:VAL:O	1:A:559:LEU:HB3	2.09	0.53
1:A:10:TYR:CZ	1:A:20:LYS:HE3	2.43	0.52
1:A:777:LEU:HD11	1:A:800:LEU:HD13	1.90	0.52
1:B:683:THR:HG23	1:B:685:ASN:CB	2.40	0.52
1:B:266:ASP:HB2	1:B:270:GLN:H	1.74	0.52
1:B:647:ARG:NE	2:B:901:HOH:O	2.04	0.52
1:A:129:PHE:HZ	1:A:162:TYR:HB2	1.74	0.52
1:A:389:VAL:O	1:A:390:ASN:HB2	2.10	0.52
1:B:816:GLN:HG2	1:B:827:THR:HG21	1.91	0.52
1:B:69:THR:HG21	1:B:147:PRO:O	2.09	0.52
1:B:389:VAL:O	1:B:390:ASN:HB2	2.08	0.52
1:A:760:LYS:HD3	1:A:795:GLU:OE2	2.10	0.52
1:B:6:LEU:HD12	2:B:971:HOH:O	2.10	0.52
1:B:509:ASN:N	2:B:905:HOH:O	2.20	0.51
1:A:683:THR:HG21	1:A:688:TYR:CE2	2.45	0.51
1:B:264:GLY:O	1:B:275:ARG:NH2	2.43	0.51
1:B:627:THR:CA	2:B:904:HOH:O	2.59	0.51
1:B:194:PHE:HE1	1:B:196:GLN:HE21	1.57	0.51
1:B:610:ARG:HD2	1:B:667:ASP:OD2	2.10	0.51
1:B:24:ARG:O	1:B:26:LYS:N	2.44	0.51
1:A:604:GLN:CD	1:A:642:MET:HE3	2.36	0.51
1:B:32:LEU:HB3	1:B:35:ILE:HD11	1.92	0.51
1:B:200:PHE:O	1:B:201:VAL:HG12	2.10	0.51
1:A:153:LYS:HG3	1:A:195:TYR:CZ	2.46	0.50
1:B:76:LYS:HD3	1:B:76:LYS:H	1.75	0.50
1:A:683:THR:HG21	1:A:688:TYR:HD2	1.75	0.50
1:B:39:TYR:CZ	1:B:54:VAL:HG22	2.46	0.50
1:B:145:LYS:NZ	2:B:921:HOH:O	2.43	0.50
1:B:640:GLU:OE2	1:B:644:LYS:HG2	2.12	0.50
1:B:351:LEU:CD2	1:B:380:ILE:CD1	2.89	0.50
1:A:847:TRP:H	1:A:847:TRP:CD1	2.27	0.50
1:A:138:LEU:HB3	2:A:921:HOH:O	2.10	0.50
1:A:54:VAL:CG2	1:A:92:GLU:HA	2.42	0.50
1:B:647:ARG:NH1	2:B:915:HOH:O	2.35	0.50
1:A:599:LYS:O	1:A:600:ASP:C	2.54	0.50
1:B:847:TRP:H	1:B:847:TRP:CD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ASN:O	1:A:853:SER:CB	2.60	0.49
1:A:432:SER:HB3	1:A:819:TYR:HA	1.94	0.49
1:A:260:ARG:HB3	1:A:304:HIS:CD2	2.47	0.49
1:A:616:ILE:O	1:A:620:VAL:HG23	2.12	0.49
1:B:152:ASP:HB3	1:B:161:PHE:HB3	1.94	0.49
1:A:349:LEU:HD21	1:A:465:LYS:HE3	1.94	0.49
1:B:19:LYS:HE3	1:B:512:ARG:NH2	2.27	0.49
1:A:852:ASN:O	1:A:853:SER:HB3	2.12	0.49
1:B:292:VAL:HG22	1:B:355:MET:HE2	1.95	0.48
1:A:314:GLY:HA3	1:A:373:THR:HA	1.94	0.48
1:A:260:ARG:HB3	1:A:304:HIS:NE2	2.28	0.48
1:B:109:ASN:HB3	1:B:237:SER:HB2	1.96	0.48
1:B:208:LEU:C	1:B:210:THR:H	2.22	0.48
1:B:602:ILE:HD11	1:B:616:ILE:HD13	1.93	0.48
1:B:616:ILE:O	1:B:620:VAL:HG23	2.15	0.47
1:A:39:TYR:CZ	1:A:54:VAL:HG22	2.49	0.47
1:A:355:MET:CE	1:A:380:ILE:HD12	2.36	0.47
1:A:504:GLU:HG2	1:A:547:SER:OG	2.15	0.47
1:B:26:LYS:NZ	2:B:926:HOH:O	2.47	0.47
1:B:563:LEU:HB3	1:B:564:PRO:HD3	1.96	0.47
1:B:59:LEU:HD11	1:B:92:GLU:HG3	1.97	0.47
1:B:96:LEU:HD13	1:B:102:PHE:HA	1.97	0.47
1:A:421:LEU:HD23	1:A:421:LEU:C	2.40	0.46
1:B:23:VAL:HG11	2:B:952:HOH:O	2.15	0.46
1:A:125:ASN:O	1:A:127:GLU:N	2.47	0.46
1:B:563:LEU:HA	1:B:566:ILE:HD12	1.97	0.46
1:B:256:ILE:HG12	1:B:308:VAL:HG22	1.98	0.46
1:A:30:TYR:HB3	1:A:79:LEU:HD22	1.96	0.46
1:A:343:MET:O	1:A:347:GLN:HG3	2.16	0.46
1:A:604:GLN:HG2	1:A:642:MET:CE	2.41	0.46
1:B:355:MET:CE	1:B:383:PHE:HZ	2.29	0.46
1:A:779:ILE:HB	1:A:780:PRO:HD3	1.98	0.46
1:B:27:ASP:HB3	1:B:29:ILE:HB	1.97	0.46
1:A:731:GLY:HA3	2:A:976:HOH:O	2.15	0.46
1:B:301:GLU:HB2	1:B:306:PHE:CE1	2.51	0.46
1:B:683:THR:HG21	1:B:688:TYR:HD2	1.80	0.45
1:A:228:TYR:OH	1:A:297:GLU:OE2	2.30	0.45
1:A:372:VAL:HG13	1:A:376:LEU:HA	1.98	0.45
1:A:647:ARG:HH11	1:A:647:ARG:CG	2.07	0.45
1:B:124:THR:HG22	1:B:128:VAL:HG11	1.98	0.45
1:B:128:VAL:HA	1:B:131:GLU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:LEU:HD11	1:B:800:LEU:HD13	1.98	0.45
1:A:52:TYR:HB2	1:A:93:PHE:O	2.16	0.45
1:A:418:PHE:HD2	1:A:466:CYS:SG	2.39	0.45
1:B:559:LEU:O	1:B:563:LEU:N	2.49	0.45
1:B:610:ARG:NH2	2:B:925:HOH:O	2.46	0.45
1:B:625:LEU:HD21	1:B:682:VAL:HG12	1.97	0.45
1:B:779:ILE:HB	1:B:780:PRO:HD3	1.98	0.45
1:B:716:ASP:HB2	1:B:720:ARG:H	1.82	0.45
1:A:558:VAL:O	1:A:559:LEU:CB	2.65	0.45
1:A:671:GLY:O	1:A:674:LEU:HB2	2.17	0.45
1:B:708:VAL:HB	1:B:709:THR:H	1.68	0.45
1:B:766:SER:HG	1:B:817:PHE:H	1.63	0.45
1:A:117:LYS:NZ	1:A:151:ASN:HD22	2.15	0.45
1:A:144:LYS:HB3	1:A:144:LYS:HE2	1.81	0.45
1:A:464:GLU:HA	1:A:467:ASP:HB2	1.98	0.45
1:B:456:TYR:CE1	1:B:460:VAL:HG21	2.51	0.44
1:B:512:ARG:HG2	1:B:527:LYS:HG2	1.99	0.44
1:B:558:VAL:O	1:B:559:LEU:HB3	2.17	0.44
1:B:420:ARG:HE	1:B:431:THR:HG22	1.82	0.44
1:A:176:GLU:OE1	1:A:178:CYS:CB	2.65	0.44
1:A:686:GLN:O	1:A:690:GLU:HG2	2.18	0.44
1:B:258:GLU:HG2	1:B:306:PHE:CE2	2.52	0.44
1:B:351:LEU:CD2	1:B:380:ILE:HD12	2.47	0.44
1:B:418:PHE:HD2	1:B:466:CYS:SG	2.40	0.44
1:B:613:LEU:HD13	1:B:642:MET:HB3	2.00	0.44
1:A:176:GLU:O	1:A:177:HIS:CB	2.62	0.44
1:A:201:VAL:O	1:A:201:VAL:HG13	2.18	0.44
1:B:355:MET:HE2	1:B:383:PHE:HZ	1.82	0.44
1:A:452:GLY:N	2:A:919:HOH:O	2.50	0.44
1:A:162:TYR:O	1:A:163:ARG:HB2	2.18	0.44
1:A:52:TYR:O	1:A:92:GLU:HG3	2.18	0.44
1:B:128:VAL:HG22	1:B:132:LEU:HD22	2.00	0.44
1:A:389:VAL:O	1:A:390:ASN:CB	2.65	0.43
1:B:647:ARG:NH2	2:B:901:HOH:O	2.51	0.43
1:B:653:LEU:HD21	2:B:915:HOH:O	2.18	0.43
1:B:68:VAL:HG22	1:B:160:VAL:HG22	2.00	0.43
1:B:168:LYS:NZ	2:B:934:HOH:O	2.51	0.43
1:B:558:VAL:O	1:B:559:LEU:CB	2.66	0.43
1:B:325:PHE:CE1	1:B:428:PRO:HD3	2.53	0.43
1:B:372:VAL:HG13	1:B:376:LEU:HA	2.01	0.43
1:A:66:ILE:HG12	1:A:133:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PHE:O	1:A:478:PRO:HD3	2.18	0.43
1:B:128:VAL:HG22	1:B:132:LEU:CD2	2.48	0.43
1:A:49:TRP:CD2	1:A:94:LYS:HE3	2.53	0.43
1:B:627:THR:C	1:B:629:ASN:N	2.77	0.43
1:A:318:ARG:HG3	1:A:367:PRO:HB2	2.00	0.43
1:A:361:ALA:HB2	1:A:389:VAL:HG12	2.00	0.42
1:A:814:PRO:HB2	1:A:818:SER:HA	2.01	0.42
1:B:361:ALA:HB2	1:B:389:VAL:HG12	2.01	0.42
1:B:456:TYR:O	1:B:460:VAL:HG23	2.20	0.42
1:B:228:TYR:OH	1:B:297:GLU:OE2	2.33	0.42
1:B:530:PHE:CD1	1:B:849:PRO:HB3	2.54	0.42
1:B:706:ASP:HB3	1:B:709:THR:O	2.19	0.42
1:B:373:THR:HG22	1:B:377:THR:CB	2.48	0.42
1:B:432:SER:HB3	1:B:819:TYR:HA	2.00	0.42
1:B:492:LEU:HD22	1:B:836:LEU:HD22	2.01	0.42
1:A:52:TYR:HE2	1:A:95:HIS:HE1	1.68	0.42
1:B:389:VAL:O	1:B:390:ASN:CB	2.68	0.42
1:B:28:ASN:OD1	1:B:28:ASN:N	2.53	0.42
1:B:492:LEU:CD2	1:B:836:LEU:HD22	2.50	0.42
1:A:227:LYS:HD3	1:A:227:LYS:HA	1.90	0.42
1:B:227:LYS:NZ	1:B:247:ARG:HD2	2.35	0.42
1:B:438:TYR:OH	1:B:807:LYS:HE2	2.19	0.42
1:A:236:PHE:HA	1:A:241:GLY:HA2	2.02	0.42
1:A:249:LYS:HD3	1:A:249:LYS:HA	1.85	0.42
1:A:163:ARG:HG3	1:A:195:TYR:CE1	2.55	0.42
1:B:600:ASP:HB3	1:B:601:ASN:H	1.49	0.42
1:A:55:LYS:NZ	1:A:90:LYS:HD3	2.36	0.41
1:B:48:VAL:HG23	1:B:49:TRP:CD1	2.55	0.41
1:B:343:MET:O	1:B:347:GLN:HG3	2.20	0.41
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.97	0.41
1:A:54:VAL:HG21	1:A:92:GLU:HA	2.03	0.41
1:A:492:LEU:HD22	1:A:836:LEU:HD22	2.01	0.41
1:A:326:PRO:O	1:A:762:ARG:NH1	2.53	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.92	0.41
1:A:96:LEU:HD13	1:A:102:PHE:HA	2.03	0.41
1:B:46:GLU:HG3	1:B:46:GLU:O	2.19	0.41
1:A:234:LEU:HB3	1:A:242:VAL:HG23	2.01	0.41
1:A:362:MET:HG3	1:A:380:ILE:HG21	2.02	0.41
1:B:132:LEU:HD13	1:B:132:LEU:HA	1.90	0.41
1:B:563:LEU:N	1:B:564:PRO:CD	2.84	0.41
1:B:6:LEU:HD23	1:B:522:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HH22	1:A:205:ASP:CG	2.29	0.41
1:A:647:ARG:NH1	2:A:924:HOH:O	2.54	0.41
1:A:412:ALA:HB1	1:A:470:ILE:HG23	2.02	0.41
1:A:468:LYS:HB3	1:A:471:LYS:HG3	2.01	0.41
1:A:563:LEU:HD23	1:A:563:LEU:HA	1.90	0.41
1:A:696:ILE:HD12	1:A:739:LEU:HD22	2.02	0.41
1:B:684:GLN:HA	1:B:684:GLN:NE2	2.36	0.41
1:A:20:LYS:HA	1:A:20:LYS:HD3	1.96	0.41
1:A:329:GLU:HA	1:A:762:ARG:NH2	2.36	0.41
1:B:420:ARG:HH21	1:B:431:THR:HB	1.86	0.41
1:B:401:GLY:O	1:B:420:ARG:HG2	2.20	0.40
1:B:24:ARG:O	1:B:25:GLY:C	2.63	0.40
1:B:697:LYS:NZ	2:B:943:HOH:O	2.55	0.40
1:B:19:LYS:HE3	1:B:512:ARG:HH22	1.86	0.40
1:B:364:ASP:O	1:B:369:ASN:ND2	2.45	0.40
1:B:600:ASP:O	1:B:601:ASN:C	2.64	0.40
1:A:32:LEU:HB2	1:A:35:ILE:HD11	2.04	0.40
1:A:54:VAL:HG21	1:A:91:ILE:C	2.47	0.40
1:B:260:ARG:HA	1:B:261:PRO:HD3	1.97	0.40
1:B:399:THR:O	1:B:400:THR:C	2.64	0.40
1:B:66:ILE:HB	1:B:121:ILE:HB	2.03	0.40
1:B:190:GLN:N	2:B:939:HOH:O	2.53	0.40
1:B:575:LYS:O	1:B:579:LEU:HG	2.21	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	825/875 (94%)	763 (92%)	49 (6%)	13 (2%)	7	13
1	B	836/875 (96%)	782 (94%)	43 (5%)	11 (1%)	9	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1661/1750 (95%)	1545 (93%)	92 (6%)	24 (1%)	9 16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	176	GLU
1	A	250	ASP
1	A	763	CYS
1	B	14	ASN
1	B	25	GLY
1	B	29	ILE
1	B	110	ALA
1	B	250	ASP
1	A	177	HIS
1	A	200	PHE
1	A	559	LEU
1	A	708	VAL
1	A	853	SER
1	B	172	ASN
1	B	559	LEU
1	B	708	VAL
1	A	156	LYS
1	A	302	TRP
1	A	34	ASP
1	B	302	TRP
1	B	600	ASP
1	A	155	TRP
1	B	249	LYS

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	741/778 (95%)	691 (93%)	50 (7%)	15 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	750/778 (96%)	716 (96%)	34 (4%)	24	46
All	All	1491/1556 (96%)	1407 (94%)	84 (6%)	19	37

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	20	LYS
1	A	37	ASP
1	A	38	THR
1	A	51	HIS
1	A	55	LYS
1	A	74	ASP
1	A	77	ASP
1	A	90	LYS
1	A	144	LYS
1	A	145	LYS
1	A	156	LYS
1	A	157	ASN
1	A	163	ARG
1	A	174	HIS
1	A	199	ASP
1	A	211	ILE
1	A	249	LYS
1	A	260	ARG
1	A	277	LYS
1	A	286	LEU
1	A	301	GLU
1	A	303	GLU
1	A	310	GLU
1	A	323	GLN
1	A	332	ASN
1	A	360	VAL
1	A	372	VAL
1	A	449	GLU
1	A	463	GLN
1	A	467	ASP
1	A	468	LYS
1	A	475	THR
1	A	481	ILE
1	A	514	ILE
1	A	546	SER

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Mol	Chain	Res	Type
1	A	595	LEU
1	A	597	ILE
1	A	647	ARG
1	A	649	LYS
1	A	655	VAL
1	A	661	VAL
1	A	663	ILE
1	A	683	THR
1	A	690	GLU
1	A	715	VAL
1	A	721	LEU
1	A	754	SER
1	A	762	ARG
1	A	766	SER
1	B	21	ILE
1	B	121	ILE
1	B	131	GLU
1	B	132	LEU
1	B	138	LEU
1	B	173	GLU
1	B	199	ASP
1	B	201	VAL
1	B	211	ILE
1	B	260	ARG
1	B	300	GLN
1	B	351	LEU
1	B	362	MET
1	B	365	LEU
1	B	372	VAL
1	B	409	VAL
1	B	431	THR
1	B	481	ILE
1	B	514	ILE
1	B	546	SER
1	B	567	GLU
1	B	595	LEU
1	B	599	LYS
1	B	650	ASP
1	B	655	VAL
1	B	661	VAL
1	B	663	ILE
1	B	673	SER

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Mol	Chain	Res	Type
1	B	683	THR
1	B	715	VAL
1	B	754	SER
1	B	765	ILE
1	B	766	SER
1	B	788	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	51	HIS
1	A	53	HIS
1	A	151	ASN
1	A	190	GLN
1	A	192	ASN
1	A	270	GLN
1	A	323	GLN
1	A	347	GLN
1	A	482	ASN
1	A	497	ASN
1	A	556	GLN
1	A	686	GLN
1	A	794	ASN
1	B	33	ASN
1	B	62	GLN
1	B	157	ASN
1	B	190	GLN
1	B	270	GLN
1	B	294	ASN
1	B	300	GLN
1	B	332	ASN
1	B	646	ASN
1	B	684	GLN
1	B	686	GLN
1	B	713	GLN
1	B	717	ASN
1	B	740	ASN
1	B	816	GLN

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	833/875 (95%)	0.17	30 (3%) 46 42	38, 88, 181, 238	0
1	B	842/875 (96%)	-0.12	6 (0%) 84 82	37, 76, 126, 196	0
All	All	1675/1750 (95%)	0.02	36 (2%) 63 60	37, 80, 168, 238	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ASN	5.0
1	A	133	LEU	4.9
1	A	68	VAL	4.0
1	B	201	VAL	3.8
1	B	211	ILE	3.4
1	A	132	LEU	3.3
1	A	302	TRP	3.2
1	A	155	TRP	3.1
1	B	302	TRP	3.1
1	A	82	VAL	3.0
1	A	119	ILE	2.9
1	A	211	ILE	2.8
1	A	136	ILE	2.7
1	A	30	TYR	2.7
1	A	201	VAL	2.6
1	A	83	ALA	2.6
1	A	200	PHE	2.5
1	A	601	ASN	2.5
1	A	79	LEU	2.5
1	A	29	ILE	2.4
1	A	170	ILE	2.3
1	A	67	HIS	2.3
1	A	135	MET	2.3
1	A	128	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	124	THR	2.2
1	B	200	PHE	2.2
1	B	602	ILE	2.2
1	A	376	LEU	2.2
1	A	481	ILE	2.2
1	A	66	ILE	2.1
1	A	208	LEU	2.1
1	A	36	PRO	2.1
1	A	425	LEU	2.1
1	A	138	LEU	2.0
1	A	653	LEU	2.0
1	B	29	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.