



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2025 – 04:28 pm GMT

PDB ID : 9G9O
Title : Lipid III flippase Wzx E with NB10 and NB7 nanobodies in outward-facing conformation - crystal 2
Authors : Le Bas, A.; Naismith, J.H.
Deposited on : 2024-07-25
Resolution : 2.69 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

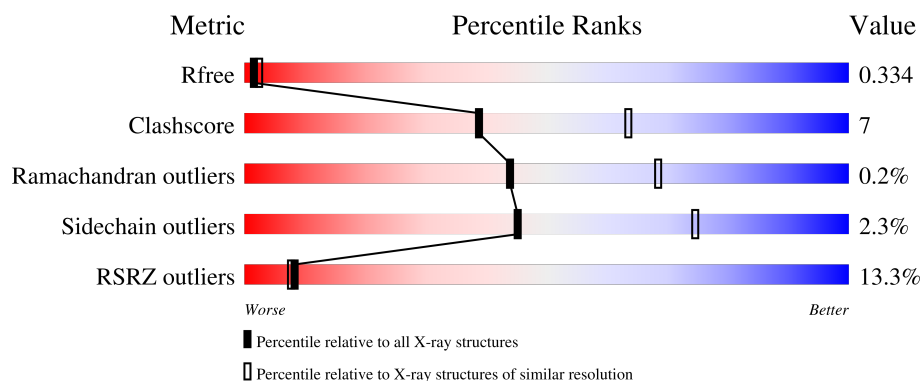
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	425	<div> <div>9%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
2	B	140	<div> <div>14%</div> <div>69%</div> <div>21%</div> <div>.</div> <div>9%</div> </div>
3	C	136	<div> <div>23%</div> <div>69%</div> <div>22%</div> <div>.</div> <div>8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5101 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 Lipid III flippase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3167	2106	516	531	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0AAA7
A	1	VAL	-	cloning artifact	UNP P0AAA7
A	417	LEU	-	expression tag	UNP P0AAA7
A	418	GLU	-	expression tag	UNP P0AAA7
A	419	GLU	-	expression tag	UNP P0AAA7
A	420	ASN	-	expression tag	UNP P0AAA7
A	421	LEU	-	expression tag	UNP P0AAA7
A	422	TYR	-	expression tag	UNP P0AAA7
A	423	PHE	-	expression tag	UNP P0AAA7
A	424	GLN	-	expression tag	UNP P0AAA7

- Molecule 2 is a protein called NB10 Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			960	597	174	185	4			

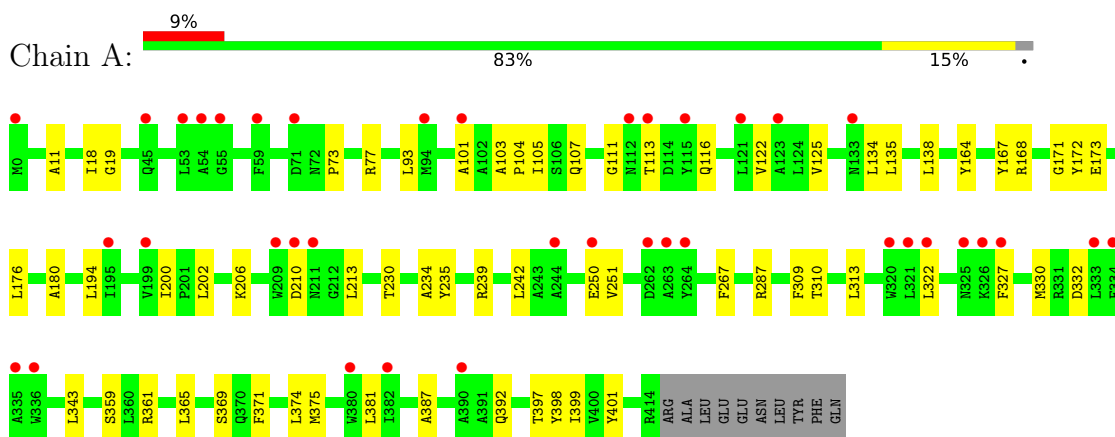
- Molecule 3 is a protein called NB7 Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	0	0
			974	615	168	186	5			

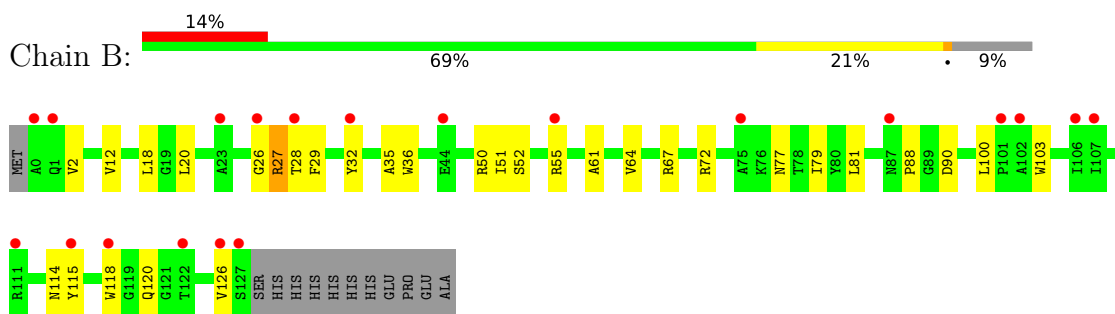
3 Residue-property plots [i](#)

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.

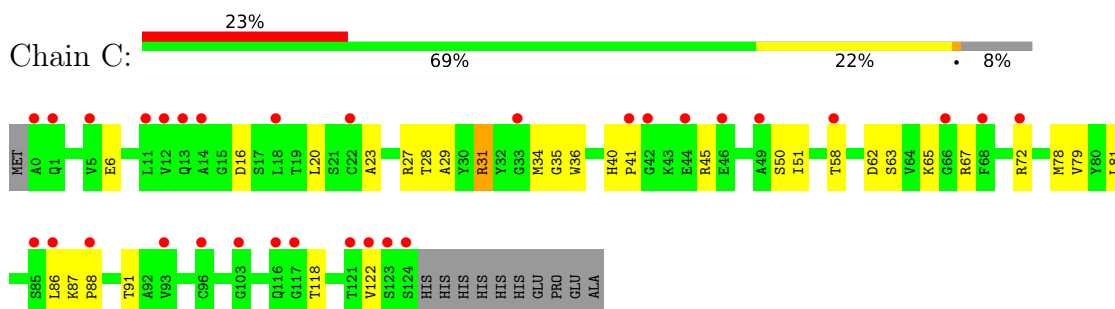
• Molecule 1: Lipid III flippase



• Molecule 2: NB10 Nanobody



• Molecule 3: NB7 Nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	42.34Å 154.02Å 288.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.50 – 2.69 38.50 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.50-2.69) 99.4 (38.50-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.279 , 0.338 0.280 , 0.334	Depositor DCC
R_{free} test set	1299 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5101	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/3239	0.43	0/4410
2	B	0.26	0/980	0.52	0/1329
3	C	0.27	0/999	0.50	0/1353
All	All	0.25	0/5218	0.46	0/7092

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3167	0	3338	37	0
2	B	960	0	930	18	0
3	C	974	0	925	17	0
All	All	5101	0	5193	69	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 7.

All (69) 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:164:TYR:OH	1:A:168:ARG:NH1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG11	1:A:180:ALA:HB1	1.77	0.65
3:C:91:THR:HG22	3:C:122:VAL:H	1.62	0.63
1:A:173:GLU:H	2:B:114:ASN:HD21	1.48	0.62
2:B:2:VAL:HG11	2:B:32:TYR:HE2	1.64	0.61
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.24	0.61
1:A:343:LEU:HD22	1:A:399:ILE:HA	1.82	0.60
2:B:52:SER:O	2:B:72:ARG:NH1	2.37	0.58
3:C:35:GLY:HA2	3:C:50:SER:HA	1.88	0.56
1:A:210:ASP:HB3	1:A:213:LEU:HB2	1.88	0.56
2:B:27:ARG:HG3	2:B:28:THR:H	1.71	0.55
2:B:20:LEU:HD12	2:B:81:LEU:HD23	1.89	0.54
3:C:28:THR:HB	3:C:31:ARG:HG3	1.89	0.54
1:A:113:THR:HG1	1:A:116:GLN:HE21	1.53	0.54
3:C:51:ILE:HG13	3:C:58:THR:HG22	1.90	0.54
1:A:327:PHE:O	1:A:330:MET:HG2	2.07	0.54
1:A:194:LEU:HD21	1:A:200:ILE:HD11	1.89	0.53
3:C:29:ALA:O	3:C:72:ARG:NH2	2.42	0.53
2:B:51:ILE:HD13	2:B:72:ARG:HB3	1.90	0.53
1:A:103:ALA:HB3	1:A:104:PRO:HD3	1.90	0.52
1:A:135:LEU:HD22	1:A:194:LEU:HD22	1.92	0.52
1:A:171:GLY:HA3	2:B:103:TRP:O	2.08	0.52
3:C:40:HIS:HB3	3:C:41:PRO:HD2	1.93	0.51
1:A:101:ALA:O	1:A:105:ILE:HG13	2.12	0.50
1:A:374:LEU:HG	1:A:397:THR:HG21	1.95	0.49
1:A:332:ASP:OD2	3:C:31:ARG:HD3	2.12	0.49
2:B:88:PRO:HA	2:B:126:VAL:HB	1.95	0.49
1:A:310:THR:HA	1:A:313:LEU:HD12	1.95	0.48
3:C:72:ARG:HG3	3:C:79:VAL:HG22	1.95	0.48
3:C:63:SER:O	3:C:67:ARG:NH1	2.47	0.47
3:C:87:LYS:HB3	3:C:88:PRO:HD2	1.96	0.47
1:A:122:VAL:HA	1:A:125:VAL:HB	1.97	0.47
2:B:29:PHE:HZ	2:B:79:ILE:HG23	1.80	0.46
2:B:27:ARG:HG3	2:B:28:THR:N	2.30	0.46
1:A:250:GLU:HG3	1:A:387:ALA:HB2	1.98	0.46
1:A:235:TYR:O	1:A:239:ARG:HG3	2.17	0.45
1:A:11:ALA:HA	1:A:267:PHE:HD1	1.83	0.44
1:A:381:LEU:HD13	1:A:392:GLN:HB2	1.99	0.44
3:C:62:ASP:HA	3:C:65:LYS:HD3	2.00	0.44
1:A:73:PRO:O	1:A:77:ARG:HG3	2.18	0.43
1:A:135:LEU:HA	1:A:138:LEU:HD12	2.01	0.43
3:C:34:MET:HG3	3:C:79:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:LEU:HD12	3:C:81:LEU:HD23	2.00	0.43
1:A:134:LEU:O	1:A:138:LEU:HG	2.19	0.43
2:B:115:TYR:O	2:B:118:TRP:NE1	2.51	0.43
2:B:12:VAL:HG21	2:B:18:LEU:HB2	2.00	0.42
2:B:61:ALA:HB3	2:B:64:VAL:HG22	2.01	0.42
3:C:6:GLU:HB3	3:C:118:THR:HG23	2.00	0.42
1:A:113:THR:OG1	1:A:116:GLN:NE2	2.43	0.42
1:A:359:SER:HA	1:A:361:ARG:NH2	2.33	0.42
1:A:107:GLN:NE2	1:A:111:GLY:O	2.53	0.42
1:A:234:ALA:HB2	1:A:371:PHE:CD2	2.54	0.42
2:B:100:LEU:HB2	2:B:103:TRP:CD1	2.54	0.42
1:A:365:LEU:O	1:A:369:SER:OG	2.28	0.42
3:C:86:LEU:HD13	3:C:86:LEU:HA	1.92	0.42
3:C:23:ALA:HA	3:C:78:MET:HG2	2.02	0.41
1:A:242:LEU:HB3	1:A:251:VAL:HG22	2.02	0.41
2:B:26:GLY:O	2:B:77:ASN:ND2	2.53	0.41
1:A:234:ALA:O	1:A:375:MET:HE3	2.20	0.41
1:A:309:PHE:O	1:A:313:LEU:HG	2.21	0.41
2:B:35:ALA:HA	2:B:50:ARG:HA	2.02	0.41
1:A:18:ILE:HG13	1:A:19:GLY:N	2.35	0.41
1:A:242:LEU:HD21	1:A:250:GLU:CG	2.51	0.41
1:A:239:ARG:HB3	1:A:251:VAL:HG11	2.03	0.41
1:A:398:TYR:HA	1:A:401:TYR:HB3	2.02	0.41
1:A:172:TYR:O	1:A:176:LEU:HG	2.20	0.40
1:A:287:ARG:NH1	1:A:287:ARG:HG2	2.35	0.40
3:C:36:TRP:HE1	3:C:79:VAL:HG12	1.87	0.40
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.36	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	413/425 (97%)	404 (98%)	8 (2%)	1 (0%)	44	68
2	B	126/140 (90%)	122 (97%)	4 (3%)	0	100	100
3	C	123/136 (90%)	119 (97%)	4 (3%)	0	100	100
All	All	662/701 (94%)	645 (97%)	16 (2%)	1 (0%)	44	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	THR

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	325/334 (97%)	320 (98%)	5 (2%)	60	83
2	B	98/109 (90%)	95 (97%)	3 (3%)	35	64
3	C	99/109 (91%)	95 (96%)	4 (4%)	27	55
All	All	522/552 (95%)	510 (98%)	12 (2%)	45	74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LEU
1	A	167	TYR
1	A	202	LEU
1	A	206	LYS
1	A	322	LEU
2	B	27	ARG
2	B	55	ARG
2	B	120	GLN
3	C	16	ASP
3	C	27	ARG
3	C	31	ARG
3	C	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [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	415/425 (97%)	0.80	38 (9%) 16 15	39, 51, 69, 82	0
2	B	128/140 (91%)	1.09	20 (15%) 6 5	40, 58, 87, 109	0
3	C	125/136 (91%)	1.45	31 (24%) 2 2	48, 66, 93, 106	0
All	All	668/701 (95%)	0.98	89 (13%) 8 8	39, 54, 81, 109	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	0	ALA	5.2
3	C	33	GLY	4.7
3	C	1	GLN	4.2
3	C	116	GLN	3.9
3	C	44	GLU	3.8
3	C	18	LEU	3.5
2	B	26	GLY	3.2
3	C	46	GLU	3.2
3	C	122	VAL	3.2
1	A	0	MET	3.2
1	A	112	ASN	3.1
2	B	0	ALA	3.1
1	A	327	PHE	3.1
2	B	32	TYR	3.1
1	A	133	ASN	3.0
2	B	102	ALA	3.0
2	B	127	SER	3.0
1	A	45	GLN	2.9
1	A	264	TYR	2.9
3	C	88	PRO	2.9
1	A	326	LYS	2.9
2	B	118	TRP	2.9
3	C	124	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	320	TRP	2.8
3	C	93	VAL	2.7
2	B	28	THR	2.7
1	A	53	LEU	2.7
1	A	333	LEU	2.7
3	C	41	PRO	2.7
3	C	14	ALA	2.7
1	A	382	ILE	2.7
3	C	85	SER	2.6
1	A	211	ASN	2.6
3	C	68	PHE	2.6
2	B	111	ARG	2.6
3	C	72	ARG	2.6
2	B	106	ILE	2.6
1	A	334	PHE	2.6
3	C	13	GLN	2.5
1	A	199	VAL	2.5
3	C	5	VAL	2.5
1	A	263	ALA	2.5
3	C	103	GLY	2.5
3	C	96	CYS	2.5
1	A	59	PHE	2.5
1	A	336	TRP	2.5
3	C	22	CYS	2.5
1	A	115	TYR	2.5
2	B	1	GLN	2.4
2	B	115	TYR	2.4
3	C	49	ALA	2.4
3	C	42	GLY	2.4
3	C	121	THR	2.4
2	B	101	PRO	2.4
1	A	101	ALA	2.3
2	B	87	ASN	2.3
2	B	55	ARG	2.3
2	B	75	ALA	2.3
1	A	113	THR	2.2
1	A	71	ASP	2.2
1	A	121	LEU	2.2
1	A	322	LEU	2.2
3	C	117	GLY	2.2
3	C	58	THR	2.2
1	A	210	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	126	VAL	2.2
1	A	55	GLY	2.2
2	B	122	THR	2.2
2	B	107	ILE	2.2
2	B	23	ALA	2.2
1	A	325	ASN	2.2
3	C	12	VAL	2.2
1	A	321	LEU	2.2
3	C	86	LEU	2.2
1	A	209	TRP	2.1
1	A	244	ALA	2.1
3	C	66	GLY	2.1
3	C	123	SER	2.1
1	A	123	ALA	2.1
1	A	335	ALA	2.1
1	A	250	GLU	2.1
2	B	44	GLU	2.1
1	A	195	ILE	2.1
1	A	54	ALA	2.1
1	A	380	TRP	2.0
1	A	94	MET	2.0
3	C	11	LEU	2.0
1	A	262	ASP	2.0
1	A	390	ALA	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 monosaccharides 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.