Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 03:43 AM EDT

PDB ID	:	4H56
Title	:	Crystal structure of the Clostridium perfringens NetB toxin in the membrane inserted form
Authors	:	Savva, C.G.; Fernandes da Costa, S.P.; Bokori-Brown, M.; Naylor, C.; Cole, A.R.; Moss, D.S.; Titball, R.W.; Basak, A.K.
Deposited on	:	2012-09-18
Resolution	:	3.90 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 (i) 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 (1)) were used in the production of this report:

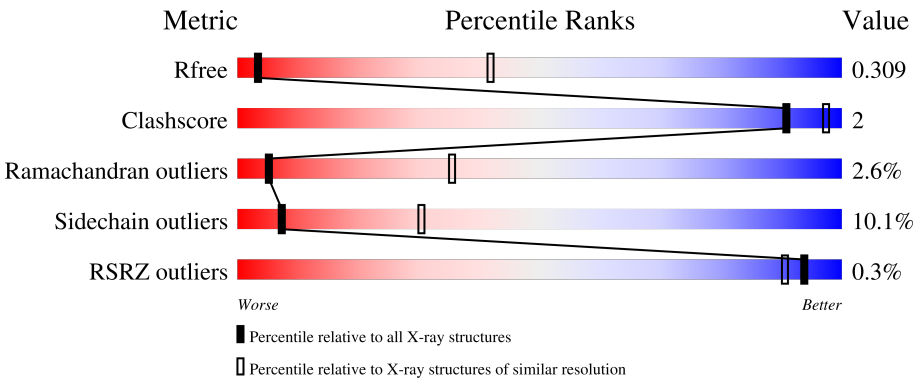
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 <=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	296	78% 11% • 10%
1	B	296	78% 11% • 10%
1	C	296	79% 10% • 10%
1	D	296	79% 10% • 10%
1	E	296	% 80% 9% • 10%

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Mol	Chain	Length	Quality of chain
1	F	296	% 77% 11% • 10%
1	G	296	% 78% 11% • 10%
1	H	296	78% 11% • 10%
1	I	296	79% 10% • 10%
1	J	296	78% 11% • 10%
1	K	296	78% 11% • 10%
1	L	296	77% 12% • 10%
1	M	296	78% 11% • 10%
1	N	296	77% 12% • 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 27963 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 Necrotic enteritis toxin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	1984	1239	335	406	4	0	0	0
1	B	267	1977	1236	328	409	4	0	0	0
1	C	267	1996	1247	337	409	3	0	0	0
1	D	267	1988	1249	331	405	3	0	0	0
1	E	267	1966	1232	331	399	4	0	0	0
1	F	267	1983	1238	330	412	3	0	0	0
1	G	267	1995	1252	331	408	4	0	0	0
1	H	267	1996	1249	335	408	4	0	0	0
1	I	267	2008	1259	336	410	3	0	0	0
1	J	267	2009	1262	336	407	4	0	0	0
1	K	267	2013	1267	334	408	4	0	0	0
1	L	267	2023	1270	336	413	4	0	0	0
1	M	267	2005	1259	332	410	4	0	0	0
1	N	267	2020	1265	337	414	4	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A8ULG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP A8ULG6
A	-1	MET	-	expression tag	UNP A8ULG6
A	0	GLY	-	expression tag	UNP A8ULG6
B	-3	GLY	-	expression tag	UNP A8ULG6
B	-2	ALA	-	expression tag	UNP A8ULG6
B	-1	MET	-	expression tag	UNP A8ULG6
B	0	GLY	-	expression tag	UNP A8ULG6
C	-3	GLY	-	expression tag	UNP A8ULG6
C	-2	ALA	-	expression tag	UNP A8ULG6
C	-1	MET	-	expression tag	UNP A8ULG6
C	0	GLY	-	expression tag	UNP A8ULG6
D	-3	GLY	-	expression tag	UNP A8ULG6
D	-2	ALA	-	expression tag	UNP A8ULG6
D	-1	MET	-	expression tag	UNP A8ULG6
D	0	GLY	-	expression tag	UNP A8ULG6
E	-3	GLY	-	expression tag	UNP A8ULG6
E	-2	ALA	-	expression tag	UNP A8ULG6
E	-1	MET	-	expression tag	UNP A8ULG6
E	0	GLY	-	expression tag	UNP A8ULG6
F	-3	GLY	-	expression tag	UNP A8ULG6
F	-2	ALA	-	expression tag	UNP A8ULG6
F	-1	MET	-	expression tag	UNP A8ULG6
F	0	GLY	-	expression tag	UNP A8ULG6
G	-3	GLY	-	expression tag	UNP A8ULG6
G	-2	ALA	-	expression tag	UNP A8ULG6
G	-1	MET	-	expression tag	UNP A8ULG6
G	0	GLY	-	expression tag	UNP A8ULG6
H	-3	GLY	-	expression tag	UNP A8ULG6
H	-2	ALA	-	expression tag	UNP A8ULG6
H	-1	MET	-	expression tag	UNP A8ULG6
H	0	GLY	-	expression tag	UNP A8ULG6
I	-3	GLY	-	expression tag	UNP A8ULG6
I	-2	ALA	-	expression tag	UNP A8ULG6
I	-1	MET	-	expression tag	UNP A8ULG6
I	0	GLY	-	expression tag	UNP A8ULG6
J	-3	GLY	-	expression tag	UNP A8ULG6
J	-2	ALA	-	expression tag	UNP A8ULG6
J	-1	MET	-	expression tag	UNP A8ULG6
J	0	GLY	-	expression tag	UNP A8ULG6
K	-3	GLY	-	expression tag	UNP A8ULG6
K	-2	ALA	-	expression tag	UNP A8ULG6
K	-1	MET	-	expression tag	UNP A8ULG6

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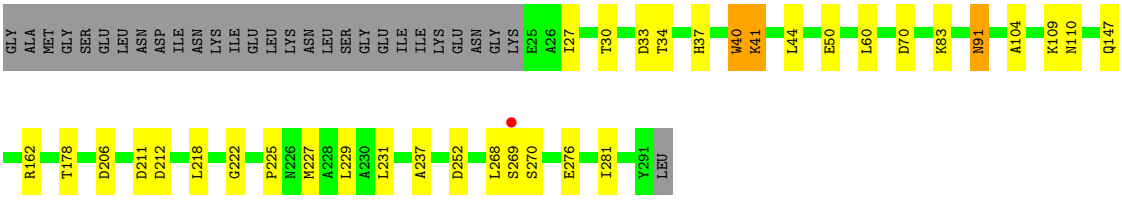
Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP A8ULG6
L	-3	GLY	-	expression tag	UNP A8ULG6
L	-2	ALA	-	expression tag	UNP A8ULG6
L	-1	MET	-	expression tag	UNP A8ULG6
L	0	GLY	-	expression tag	UNP A8ULG6
M	-3	GLY	-	expression tag	UNP A8ULG6
M	-2	ALA	-	expression tag	UNP A8ULG6
M	-1	MET	-	expression tag	UNP A8ULG6
M	0	GLY	-	expression tag	UNP A8ULG6
N	-3	GLY	-	expression tag	UNP A8ULG6
N	-2	ALA	-	expression tag	UNP A8ULG6
N	-1	MET	-	expression tag	UNP A8ULG6
N	0	GLY	-	expression tag	UNP A8ULG6

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.

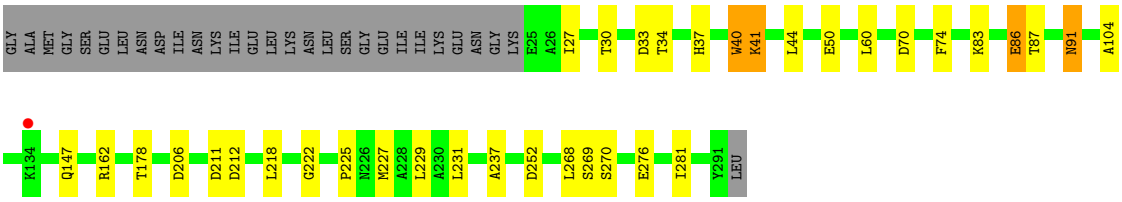
• Molecule 1: Necrotic enteritis toxin B

Chain A: 78% 11% • 10%



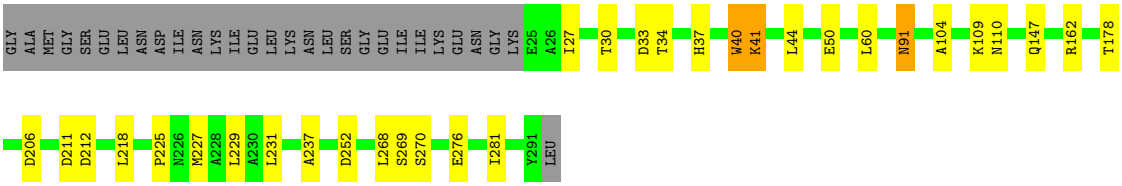
• Molecule 1: Necrotic enteritis toxin B

Chain B: 78% 11% • 10%



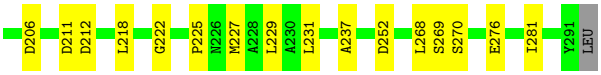
• Molecule 1: Necrotic enteritis toxin B

Chain C: 79% 10% • 10%



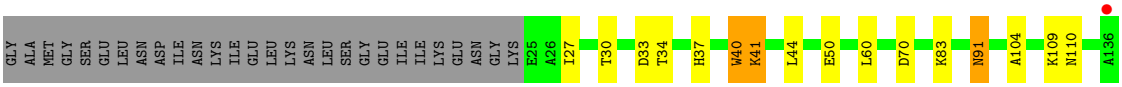
• Molecule 1: Necrotic enteritis toxin B

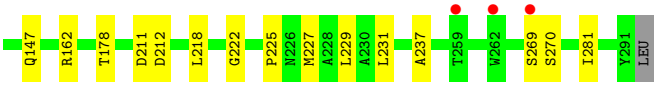
Chain D: 79% 10% • 10%



• Molecule 1: Necrotic enteritis toxin B

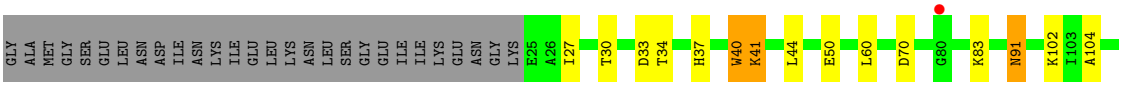
Chain E:

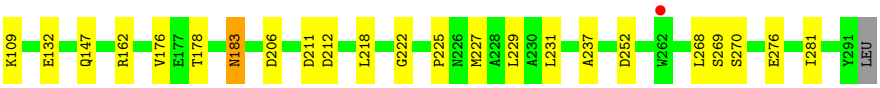




• Molecule 1: Necrotic enteritis toxin B

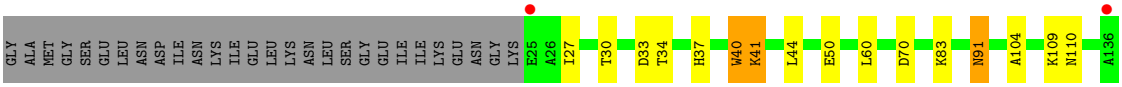
Chain F:





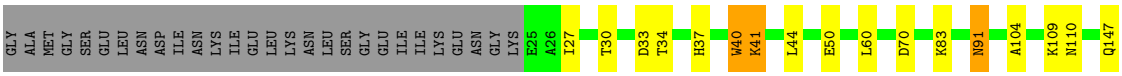
• Molecule 1: Necrotic enteritis toxin B

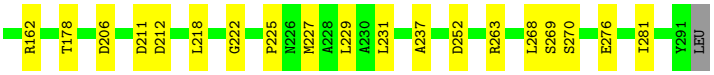
Chain G:



• Molecule 1: Necrotic enteritis toxin B

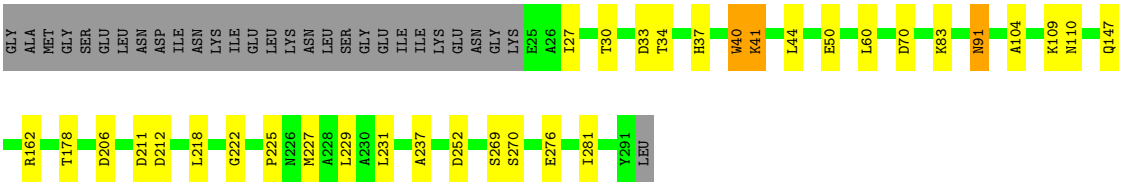
Chain H:





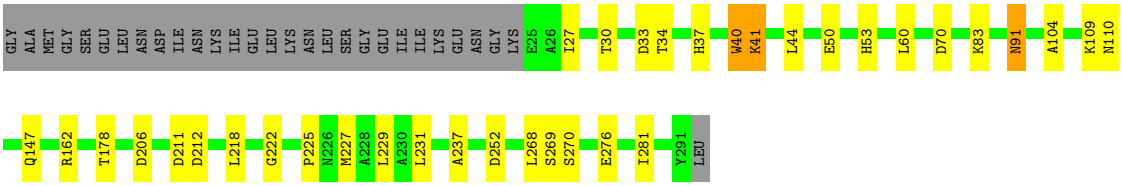
• Molecule 1: Necrotic enteritis toxin B

Chain I:



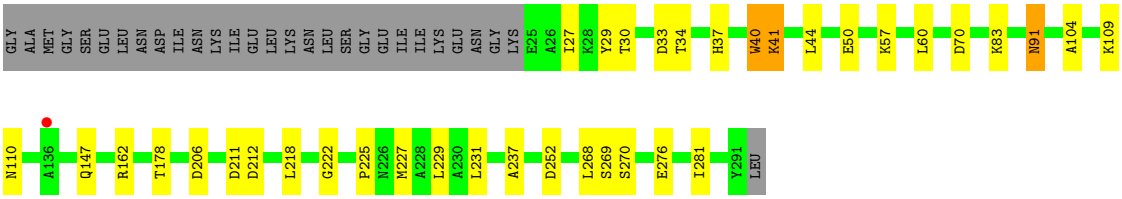
• Molecule 1: Necrotic enteritis toxin B

Chain J:



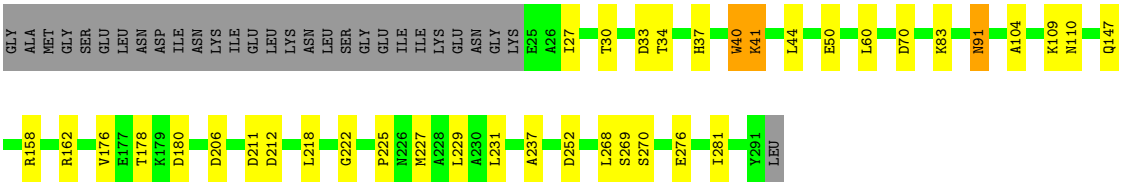
• Molecule 1: Necrotic enteritis toxin B

Chain K:



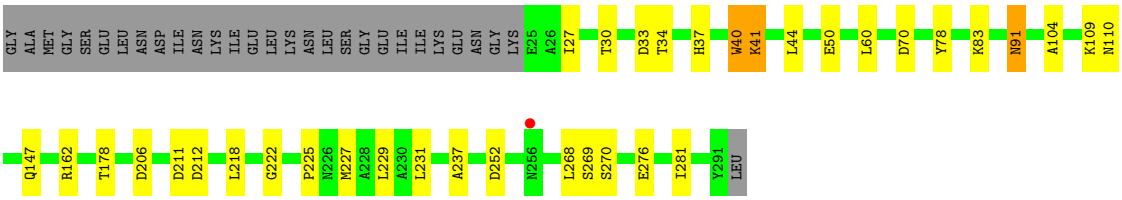
• Molecule 1: Necrotic enteritis toxin B

Chain L:



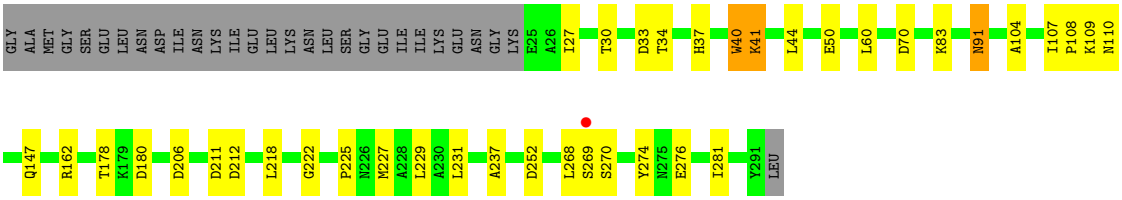
• Molecule 1: Necrotic enteritis toxin B

Chain M:



• Molecule 1: Necrotic enteritis toxin B

Chain N:


GLY
ALA
MET
GLY
SER
GLU
LEU
ASN
ASP
ILE
ASN
LYS
ILE
GLU
LEU
LYS
ASN
LEU
SER
GLY
GLU
ILE
ILE
LYS
GLU
ASN
GLY
LYS
E25
A26
I27
T30
D33
T34
H37
W40
K41
L44
E50
L60
D70
K83
N91
A104
I107
P108
K109
N110
Q147
R162
T178
K179
D180
D206
D211
D212
L218
G222
P225
N226
M227
A228
L229
A230
L231
A237
D252
L268
S269
S270
Y274
N275
E276
I281
Y291
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	313.23Å 168.04Å 160.46Å 90.00° 109.42° 90.00°	Depositor
Resolution (Å)	27.70 – 3.90 27.71 – 3.90	Depositor EDS
% Data completeness (in resolution range)	89.6 (27.70-3.90) 97.5 (27.71-3.90)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 3.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.284 , 0.309 0.284 , 0.309	Depositor DCC
R_{free} test set	3514 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	1.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 61.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	27963	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.23	0/2025	0.46	0/2763
1	B	0.23	0/2019	0.47	0/2761
1	C	0.23	0/2039	0.47	0/2785
1	D	0.23	0/2033	0.46	0/2779
1	E	0.23	0/2009	0.46	0/2747
1	F	0.24	0/2025	0.47	0/2767
1	G	0.23	0/2040	0.46	0/2788
1	H	0.23	0/2040	0.47	0/2786
1	I	0.24	0/2053	0.46	0/2802
1	J	0.23	0/2053	0.46	0/2798
1	K	0.23	0/2058	0.46	0/2805
1	L	0.24	0/2068	0.48	1/2820 (0.0%)
1	M	0.24	0/2051	0.47	0/2803
1	N	0.23	0/2064	0.47	1/2815 (0.0%)
All	All	0.23	0/28577	0.47	2/39019 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	180	ASP	CB-CG-OD2	5.22	123.00	118.30
1	N	180	ASP	CB-CG-OD2	5.17	122.95	118.30

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	1984	0	1765	7	0
1	B	1977	0	1728	8	0
1	C	1996	0	1765	5	0
1	D	1988	0	1748	6	0
1	E	1966	0	1721	7	0
1	F	1983	0	1737	8	0
1	G	1995	0	1754	7	0
1	H	1996	0	1760	8	0
1	I	2008	0	1781	7	0
1	J	2009	0	1804	9	0
1	K	2013	0	1809	9	0
1	L	2023	0	1815	9	0
1	M	2005	0	1765	7	0
1	N	2020	0	1809	9	0
All	All	27963	0	24761	90	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 2.

All (90) 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:F:183:ASN:OD1	1:G:213:ARG:NE	2.24	0.70
1:F:176:VAL:O	1:F:183:ASN:ND2	2.27	0.68
1:C:110:ASN:ND2	1:D:222:GLY:O	2.35	0.60
1:B:74:PHE:HB3	1:N:274:TYR:CG	2.39	0.57
1:M:110:ASN:ND2	1:N:222:GLY:O	2.40	0.54
1:H:222:GLY:O	1:N:110:ASN:ND2	2.40	0.54
1:A:222:GLY:O	1:G:110:ASN:ND2	2.42	0.53
1:F:91:ASN:OD1	1:F:91:ASN:N	2.43	0.52
1:M:91:ASN:N	1:M:91:ASN:OD1	2.43	0.52
1:A:91:ASN:N	1:A:91:ASN:OD1	2.43	0.52
1:C:91:ASN:N	1:C:91:ASN:OD1	2.43	0.52
1:B:91:ASN:OD1	1:B:91:ASN:N	2.43	0.52
1:L:91:ASN:N	1:L:91:ASN:OD1	2.43	0.52
1:E:91:ASN:N	1:E:91:ASN:OD1	2.43	0.51
1:N:91:ASN:N	1:N:91:ASN:OD1	2.43	0.51
1:D:91:ASN:N	1:D:91:ASN:OD1	2.43	0.51
1:H:91:ASN:N	1:H:91:ASN:OD1	2.43	0.51
1:K:91:ASN:N	1:K:91:ASN:OD1	2.43	0.51
1:G:91:ASN:N	1:G:91:ASN:OD1	2.43	0.51
1:J:91:ASN:OD1	1:J:91:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ASN:ND2	1:F:222:GLY:O	2.44	0.50
1:D:110:ASN:ND2	1:E:222:GLY:O	2.44	0.49
1:L:158:ARG:HG2	1:L:176:VAL:HG21	1.95	0.49
1:N:107:ILE:HG23	1:N:108:PRO:HA	1.95	0.48
1:I:91:ASN:N	1:I:91:ASN:OD1	2.46	0.48
1:A:110:ASN:ND2	1:B:222:GLY:O	2.48	0.46
1:J:110:ASN:ND2	1:K:222:GLY:O	2.48	0.46
1:I:110:ASN:ND2	1:J:222:GLY:O	2.49	0.46
1:N:211:ASP:OD1	1:N:212:ASP:N	2.50	0.45
1:C:211:ASP:OD1	1:C:212:ASP:N	2.51	0.44
1:D:211:ASP:OD1	1:D:212:ASP:N	2.51	0.44
1:H:263:ARG:O	1:H:263:ARG:HG3	2.16	0.44
1:L:158:ARG:HG2	1:L:176:VAL:CG2	2.47	0.44
1:M:211:ASP:OD1	1:M:212:ASP:N	2.51	0.44
1:G:211:ASP:OD1	1:G:212:ASP:N	2.51	0.44
1:F:211:ASP:OD1	1:F:212:ASP:N	2.50	0.44
1:E:70:ASP:OD1	1:E:83:LYS:NZ	2.51	0.44
1:N:70:ASP:OD1	1:N:83:LYS:NZ	2.51	0.44
1:F:40:TRP:O	1:F:41:LYS:CB	2.66	0.44
1:A:211:ASP:OD1	1:A:212:ASP:N	2.51	0.44
1:B:211:ASP:OD1	1:B:212:ASP:N	2.51	0.44
1:J:70:ASP:OD1	1:J:83:LYS:NZ	2.51	0.44
1:F:70:ASP:OD1	1:F:83:LYS:NZ	2.51	0.44
1:G:70:ASP:OD1	1:G:83:LYS:NZ	2.51	0.44
1:H:70:ASP:OD1	1:H:83:LYS:NZ	2.51	0.44
1:L:70:ASP:OD1	1:L:83:LYS:NZ	2.51	0.44
1:A:33:ASP:OD1	1:A:34:THR:N	2.51	0.43
1:H:211:ASP:OD1	1:H:212:ASP:N	2.51	0.43
1:I:70:ASP:OD1	1:I:83:LYS:NZ	2.51	0.43
1:J:211:ASP:OD1	1:J:212:ASP:N	2.51	0.43
1:E:211:ASP:OD1	1:E:212:ASP:N	2.51	0.43
1:K:70:ASP:OD1	1:K:83:LYS:NZ	2.51	0.43
1:L:211:ASP:OD1	1:L:212:ASP:N	2.51	0.43
1:C:33:ASP:OD1	1:C:34:THR:N	2.52	0.43
1:E:40:TRP:O	1:E:41:LYS:CB	2.66	0.43
1:K:211:ASP:OD1	1:K:212:ASP:N	2.50	0.43
1:B:70:ASP:OD1	1:B:83:LYS:NZ	2.51	0.43
1:F:33:ASP:OD1	1:F:34:THR:N	2.51	0.43
1:G:33:ASP:OD1	1:G:34:THR:N	2.52	0.43
1:M:70:ASP:OD1	1:M:83:LYS:NZ	2.51	0.43
1:B:33:ASP:OD1	1:B:34:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:TRP:O	1:G:41:LYS:CB	2.66	0.43
1:H:40:TRP:O	1:H:41:LYS:CB	2.66	0.43
1:I:33:ASP:OD1	1:I:34:THR:N	2.52	0.43
1:I:211:ASP:OD1	1:I:212:ASP:N	2.51	0.43
1:M:33:ASP:OD1	1:M:34:THR:N	2.52	0.43
1:A:70:ASP:OD1	1:A:83:LYS:NZ	2.51	0.43
1:K:110:ASN:ND2	1:L:222:GLY:O	2.52	0.43
1:L:33:ASP:OD1	1:L:34:THR:N	2.52	0.43
1:J:33:ASP:OD1	1:J:34:THR:N	2.52	0.42
1:K:33:ASP:OD1	1:K:34:THR:N	2.52	0.42
1:N:33:ASP:OD1	1:N:34:THR:N	2.52	0.42
1:B:86:GLU:HG3	1:B:87:THR:HG22	2.01	0.42
1:C:40:TRP:O	1:C:41:LYS:CB	2.66	0.42
1:D:33:ASP:OD1	1:D:34:THR:N	2.51	0.42
1:E:33:ASP:OD1	1:E:34:THR:N	2.52	0.42
1:H:33:ASP:OD1	1:H:34:THR:N	2.52	0.42
1:H:110:ASN:ND2	1:I:222:GLY:O	2.52	0.42
1:J:53:HIS:CD2	1:K:29:TYR:CE2	3.08	0.42
1:J:53:HIS:HB3	1:K:29:TYR:HA	2.01	0.42
1:L:110:ASN:ND2	1:M:222:GLY:O	2.53	0.42
1:L:40:TRP:O	1:L:41:LYS:CB	2.68	0.41
1:N:40:TRP:O	1:N:41:LYS:CB	2.68	0.41
1:A:40:TRP:O	1:A:41:LYS:CB	2.69	0.41
1:D:40:TRP:O	1:D:41:LYS:CB	2.68	0.41
1:J:40:TRP:O	1:J:41:LYS:CB	2.68	0.41
1:K:40:TRP:O	1:K:41:LYS:CB	2.68	0.41
1:B:40:TRP:O	1:B:41:LYS:CB	2.69	0.41
1:M:40:TRP:O	1:M:41:LYS:CB	2.69	0.40
1:I:40:TRP:O	1:I:41:LYS:CB	2.68	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	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	5 35
1	B	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	5 35
1	C	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	5 35
1	D	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	5 35
1	E	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	5 35
1	F	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	5 35
1	G	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	5 35
1	H	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	5 35
1	I	265/296 (90%)	237 (89%)	21 (8%)	7 (3%)	5 35
1	J	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	5 35
1	K	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	5 35
1	L	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	5 35
1	M	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	5 35
1	N	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	5 35
All	All	3710/4144 (90%)	3297 (89%)	315 (8%)	98 (3%)	5 35

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	269	SER
1	B	41	LYS
1	B	269	SER
1	C	41	LYS
1	C	269	SER
1	D	41	LYS
1	D	269	SER
1	E	41	LYS
1	E	269	SER
1	F	37	HIS
1	F	41	LYS
1	F	269	SER
1	G	41	LYS
1	G	269	SER
1	H	41	LYS
1	H	269	SER
1	I	37	HIS
1	I	41	LYS

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Mol	Chain	Res	Type
1	I	269	SER
1	J	41	LYS
1	J	269	SER
1	K	41	LYS
1	K	269	SER
1	L	41	LYS
1	L	269	SER
1	M	41	LYS
1	M	269	SER
1	N	41	LYS
1	N	269	SER
1	A	37	HIS
1	A	237	ALA
1	B	37	HIS
1	B	237	ALA
1	C	37	HIS
1	C	237	ALA
1	D	37	HIS
1	D	237	ALA
1	E	37	HIS
1	E	237	ALA
1	F	237	ALA
1	G	37	HIS
1	G	237	ALA
1	H	37	HIS
1	H	237	ALA
1	I	237	ALA
1	J	37	HIS
1	J	237	ALA
1	K	37	HIS
1	K	237	ALA
1	L	37	HIS
1	L	237	ALA
1	M	37	HIS
1	M	237	ALA
1	N	37	HIS
1	N	237	ALA
1	A	40	TRP
1	A	104	ALA
1	B	40	TRP
1	B	104	ALA
1	C	40	TRP

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Mol	Chain	Res	Type
1	C	104	ALA
1	D	40	TRP
1	D	104	ALA
1	E	40	TRP
1	E	104	ALA
1	F	40	TRP
1	F	104	ALA
1	G	40	TRP
1	G	104	ALA
1	H	40	TRP
1	H	104	ALA
1	I	40	TRP
1	I	104	ALA
1	J	40	TRP
1	J	104	ALA
1	K	40	TRP
1	K	104	ALA
1	L	40	TRP
1	L	104	ALA
1	M	40	TRP
1	M	104	ALA
1	N	40	TRP
1	N	104	ALA
1	A	225	PRO
1	B	225	PRO
1	C	225	PRO
1	D	225	PRO
1	E	225	PRO
1	F	225	PRO
1	G	225	PRO
1	H	225	PRO
1	I	225	PRO
1	J	225	PRO
1	K	225	PRO
1	L	225	PRO
1	M	225	PRO
1	N	225	PRO

5.3.2 Protein sidechains (i)

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	197/258 (76%)	177 (90%)	20 (10%)	7	30
1	B	194/258 (75%)	174 (90%)	20 (10%)	7	30
1	C	198/258 (77%)	178 (90%)	20 (10%)	7	30
1	D	195/258 (76%)	175 (90%)	20 (10%)	7	30
1	E	190/258 (74%)	174 (92%)	16 (8%)	11	39
1	F	196/258 (76%)	173 (88%)	23 (12%)	5	26
1	G	197/258 (76%)	177 (90%)	20 (10%)	7	30
1	H	197/258 (76%)	177 (90%)	20 (10%)	7	30
1	I	200/258 (78%)	181 (90%)	19 (10%)	8	33
1	J	201/258 (78%)	181 (90%)	20 (10%)	7	30
1	K	202/258 (78%)	181 (90%)	21 (10%)	7	29
1	L	205/258 (80%)	185 (90%)	20 (10%)	8	31
1	M	199/258 (77%)	178 (89%)	21 (11%)	6	29
1	N	205/258 (80%)	185 (90%)	20 (10%)	8	31
All	All	2776/3612 (77%)	2496 (90%)	280 (10%)	7	30

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	30	THR
1	A	44	LEU
1	A	50	GLU
1	A	60	LEU
1	A	91	ASN
1	A	109	LYS
1	A	147	GLN
1	A	162	ARG
1	A	178	THR
1	A	206	ASP
1	A	218	LEU
1	A	227	MET
1	A	229	LEU
1	A	231	LEU

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Mol	Chain	Res	Type
1	A	252	ASP
1	A	268	LEU
1	A	270	SER
1	A	276	GLU
1	A	281	ILE
1	B	27	ILE
1	B	30	THR
1	B	44	LEU
1	B	50	GLU
1	B	60	LEU
1	B	86	GLU
1	B	91	ASN
1	B	147	GLN
1	B	162	ARG
1	B	178	THR
1	B	206	ASP
1	B	218	LEU
1	B	227	MET
1	B	229	LEU
1	B	231	LEU
1	B	252	ASP
1	B	268	LEU
1	B	270	SER
1	B	276	GLU
1	B	281	ILE
1	C	27	ILE
1	C	30	THR
1	C	44	LEU
1	C	50	GLU
1	C	60	LEU
1	C	91	ASN
1	C	109	LYS
1	C	147	GLN
1	C	162	ARG
1	C	178	THR
1	C	206	ASP
1	C	218	LEU
1	C	227	MET
1	C	229	LEU
1	C	231	LEU
1	C	252	ASP
1	C	268	LEU

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Mol	Chain	Res	Type
1	C	270	SER
1	C	276	GLU
1	C	281	ILE
1	D	27	ILE
1	D	30	THR
1	D	44	LEU
1	D	50	GLU
1	D	60	LEU
1	D	77	LYS
1	D	91	ASN
1	D	109	LYS
1	D	147	GLN
1	D	162	ARG
1	D	206	ASP
1	D	218	LEU
1	D	227	MET
1	D	229	LEU
1	D	231	LEU
1	D	252	ASP
1	D	268	LEU
1	D	270	SER
1	D	276	GLU
1	D	281	ILE
1	E	27	ILE
1	E	30	THR
1	E	44	LEU
1	E	50	GLU
1	E	60	LEU
1	E	91	ASN
1	E	109	LYS
1	E	147	GLN
1	E	162	ARG
1	E	178	THR
1	E	218	LEU
1	E	227	MET
1	E	229	LEU
1	E	231	LEU
1	E	270	SER
1	E	281	ILE
1	F	27	ILE
1	F	30	THR
1	F	44	LEU

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Mol	Chain	Res	Type
1	F	50	GLU
1	F	60	LEU
1	F	91	ASN
1	F	102	LYS
1	F	109	LYS
1	F	132	GLU
1	F	147	GLN
1	F	162	ARG
1	F	178	THR
1	F	183	ASN
1	F	206	ASP
1	F	218	LEU
1	F	227	MET
1	F	229	LEU
1	F	231	LEU
1	F	252	ASP
1	F	268	LEU
1	F	270	SER
1	F	276	GLU
1	F	281	ILE
1	G	27	ILE
1	G	30	THR
1	G	44	LEU
1	G	50	GLU
1	G	60	LEU
1	G	91	ASN
1	G	109	LYS
1	G	147	GLN
1	G	162	ARG
1	G	178	THR
1	G	206	ASP
1	G	218	LEU
1	G	227	MET
1	G	229	LEU
1	G	231	LEU
1	G	252	ASP
1	G	268	LEU
1	G	270	SER
1	G	276	GLU
1	G	281	ILE
1	H	27	ILE
1	H	30	THR

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Mol	Chain	Res	Type
1	H	44	LEU
1	H	50	GLU
1	H	60	LEU
1	H	91	ASN
1	H	109	LYS
1	H	147	GLN
1	H	162	ARG
1	H	178	THR
1	H	206	ASP
1	H	218	LEU
1	H	227	MET
1	H	229	LEU
1	H	231	LEU
1	H	252	ASP
1	H	268	LEU
1	H	270	SER
1	H	276	GLU
1	H	281	ILE
1	I	27	ILE
1	I	30	THR
1	I	44	LEU
1	I	50	GLU
1	I	60	LEU
1	I	91	ASN
1	I	109	LYS
1	I	147	GLN
1	I	162	ARG
1	I	178	THR
1	I	206	ASP
1	I	218	LEU
1	I	227	MET
1	I	229	LEU
1	I	231	LEU
1	I	252	ASP
1	I	270	SER
1	I	276	GLU
1	I	281	ILE
1	J	27	ILE
1	J	30	THR
1	J	44	LEU
1	J	50	GLU
1	J	60	LEU

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Mol	Chain	Res	Type
1	J	91	ASN
1	J	109	LYS
1	J	147	GLN
1	J	162	ARG
1	J	178	THR
1	J	206	ASP
1	J	218	LEU
1	J	227	MET
1	J	229	LEU
1	J	231	LEU
1	J	252	ASP
1	J	268	LEU
1	J	270	SER
1	J	276	GLU
1	J	281	ILE
1	K	27	ILE
1	K	30	THR
1	K	44	LEU
1	K	50	GLU
1	K	57	LYS
1	K	60	LEU
1	K	91	ASN
1	K	109	LYS
1	K	147	GLN
1	K	162	ARG
1	K	178	THR
1	K	206	ASP
1	K	218	LEU
1	K	227	MET
1	K	229	LEU
1	K	231	LEU
1	K	252	ASP
1	K	268	LEU
1	K	270	SER
1	K	276	GLU
1	K	281	ILE
1	L	27	ILE
1	L	30	THR
1	L	44	LEU
1	L	50	GLU
1	L	60	LEU
1	L	91	ASN

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Mol	Chain	Res	Type
1	L	109	LYS
1	L	147	GLN
1	L	162	ARG
1	L	178	THR
1	L	206	ASP
1	L	218	LEU
1	L	227	MET
1	L	229	LEU
1	L	231	LEU
1	L	252	ASP
1	L	268	LEU
1	L	270	SER
1	L	276	GLU
1	L	281	ILE
1	M	27	ILE
1	M	30	THR
1	M	44	LEU
1	M	50	GLU
1	M	60	LEU
1	M	78	TYR
1	M	91	ASN
1	M	109	LYS
1	M	147	GLN
1	M	162	ARG
1	M	178	THR
1	M	206	ASP
1	M	218	LEU
1	M	227	MET
1	M	229	LEU
1	M	231	LEU
1	M	252	ASP
1	M	268	LEU
1	M	270	SER
1	M	276	GLU
1	M	281	ILE
1	N	27	ILE
1	N	30	THR
1	N	44	LEU
1	N	50	GLU
1	N	60	LEU
1	N	91	ASN
1	N	109	LYS

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Mol	Chain	Res	Type
1	N	147	GLN
1	N	162	ARG
1	N	178	THR
1	N	206	ASP
1	N	218	LEU
1	N	227	MET
1	N	229	LEU
1	N	231	LEU
1	N	252	ASP
1	N	268	LEU
1	N	270	SER
1	N	276	GLU
1	N	281	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	53	HIS
1	M	53	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 monosaccharides 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	267/296 (90%)	-0.25	1 (0%)	92	87	3, 61, 120, 283	0
1	B	267/296 (90%)	-0.16	1 (0%)	92	87	23, 70, 128, 261	0
1	C	267/296 (90%)	-0.15	0	100	100	13, 78, 135, 315	0
1	D	267/296 (90%)	-0.03	0	100	100	28, 89, 137, 213	0
1	E	267/296 (90%)	0.04	4 (1%)	73	64	36, 91, 155, 249	0
1	F	267/296 (90%)	0.02	2 (0%)	87	82	18, 84, 140, 260	0
1	G	267/296 (90%)	-0.09	2 (0%)	87	82	18, 70, 131, 170	0
1	H	267/296 (90%)	-0.23	0	100	100	21, 67, 124, 284	0
1	I	267/296 (90%)	-0.13	0	100	100	15, 69, 117, 180	0
1	J	267/296 (90%)	-0.26	0	100	100	6, 67, 114, 214	0
1	K	267/296 (90%)	-0.25	1 (0%)	92	87	3, 59, 117, 239	0
1	L	267/296 (90%)	-0.28	0	100	100	2, 56, 108, 168	0
1	M	267/296 (90%)	-0.24	1 (0%)	92	87	9, 59, 114, 292	0
1	N	267/296 (90%)	-0.18	1 (0%)	92	87	4, 70, 126, 227	0
All	All	3738/4144 (90%)	-0.16	13 (0%)	94	90	2, 71, 132, 315	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	136	ALA	3.9
1	F	80	GLY	3.0
1	E	136	ALA	2.8
1	F	262	TRP	2.8
1	E	269	SER	2.6
1	K	136	ALA	2.6
1	B	134	LYS	2.4
1	E	259	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	269	SER	2.2
1	N	269	SER	2.2
1	G	25	GLU	2.1
1	M	256	ASN	2.1
1	E	262	TRP	2.1

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

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

6.3 Carbohydrates (i)

There are no 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.