Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 11:26 AM EDT

PDB ID	:	3SXL
Title	:	SEX-LETHAL RNA RECOGNITION DOMAINS 1 AND 2 FROM DROSOPHILA MELANOGASTER
Authors	:	Crowder, S.M.; Kanaar, R.; Rio, D.C.; Alber, T.C.
Deposited on	:	1999-04-04
Resolution	:	2.70 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 following versions of software and data (see references (i)) were used in the production of this report:

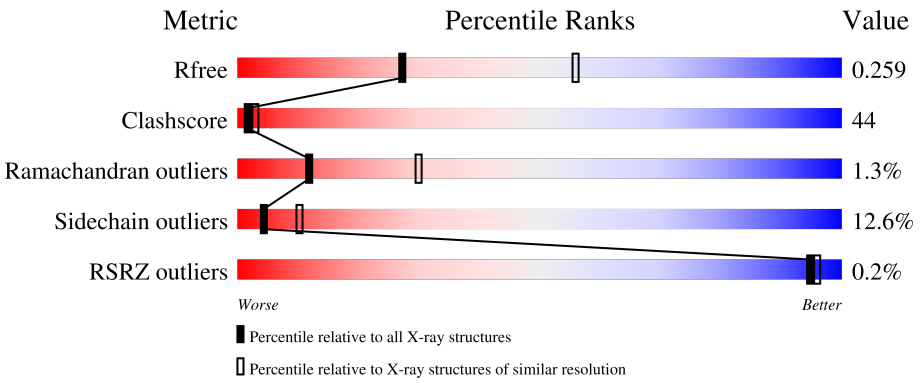
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	184	.% 29% 50% 5% • 15%
1	B	184	31% 47% 5% • 15%
1	C	184	30% 49% 5% • 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3696 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 PROTEIN (SEX-LETHAL).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	157	1232	778	217	232	1	4	0	1	0
1	B	157	1232	778	217	232	1	4	0	1	0
1	C	157	1232	778	217	232	1	4	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

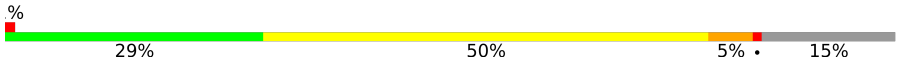
Chain	Residue	Modelled	Actual	Comment	Reference
A	111	MSE	GLN	engineered mutation	UNP P19339
A	136	MSE	MET	engineered mutation	UNP P19339
A	157	MSE	MET	engineered mutation	UNP P19339
A	177	MSE	MET	engineered mutation	UNP P19339
B	111	MSE	GLN	engineered mutation	UNP P19339
B	136	MSE	MET	engineered mutation	UNP P19339
B	157	MSE	MET	engineered mutation	UNP P19339
B	177	MSE	MET	engineered mutation	UNP P19339
C	111	MSE	GLN	engineered mutation	UNP P19339
C	136	MSE	MET	engineered mutation	UNP P19339
C	157	MSE	MET	engineered mutation	UNP P19339
C	177	MSE	MET	engineered mutation	UNP P19339

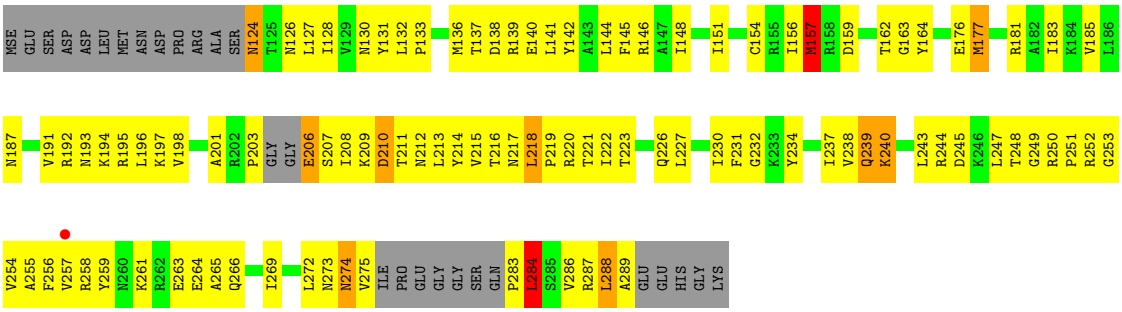
3 Residue-property plots (i)

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: PROTEIN (SEX-LETHAL)

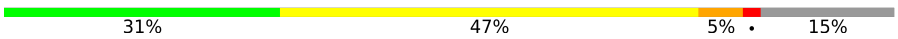
Chain A:

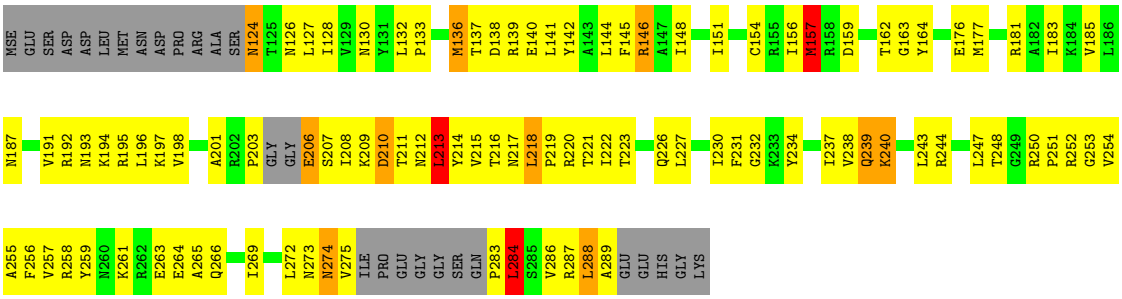




• Molecule 1: PROTEIN (SEX-LETHAL)

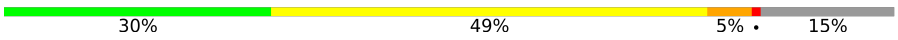
Chain B:

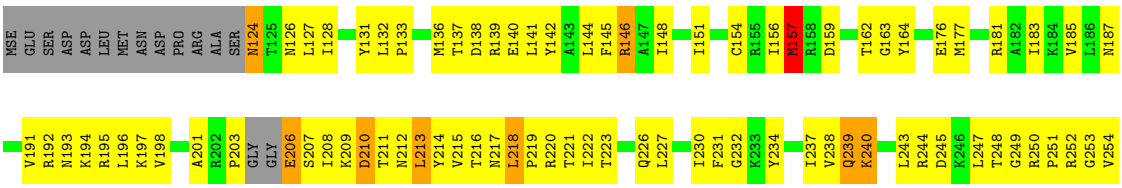


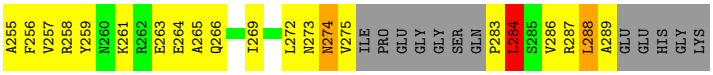


• Molecule 1: PROTEIN (SEX-LETHAL)

Chain C:






A255
F256
V257
R258
Y259
N260
K261
R262
E263
E264
A265
Q266
I269
L272
N273
N274
V275
ILE
PRO
GLU
GLY
GLY
SER
GLN
P283
L284
S285
V286
R287
L288
A289
GLU
GLU
HIS
GLY
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.91Å 124.47Å 50.93Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 21.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.70) 98.6 (21.71-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.07 (at 2.60Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.221 , 0.264 0.218 , 0.259	Depositor DCC
R_{free} test set	1674 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.470 for l,k,-h-l 0.470 for -h-l,k,h 0.088 for h,-k,-h-l 0.087 for l,-k,h 0.085 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3696	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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	0.77	3/1246 (0.2%)	0.95	3/1682 (0.2%)
1	B	0.75	2/1246 (0.2%)	0.96	3/1682 (0.2%)
1	C	0.72	1/1246 (0.1%)	0.96	3/1682 (0.2%)
All	All	0.75	6/3738 (0.2%)	0.95	9/5046 (0.2%)

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	A	0	1
1	C	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	MSE	CG-SE	-5.93	1.75	1.95
1	A	157	MSE	CG-SE	-5.92	1.75	1.95
1	C	157	MSE	CG-SE	-5.62	1.76	1.95
1	A	177[A]	MSE	CG-SE	-5.55	1.76	1.95
1	A	177[B]	MSE	CG-SE	-5.55	1.76	1.95
1	B	136	MSE	CG-SE	-5.04	1.78	1.95

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	213	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	213	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	218	LEU	CA-CB-CG	5.26	127.39	115.30
1	C	218	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	213	LEU	CA-CB-CG	5.23	127.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	LEU	CA-CB-CG	5.19	127.25	115.30
1	C	272	LEU	N-CA-C	5.13	124.85	111.00
1	A	272	LEU	N-CA-C	5.11	124.80	111.00
1	B	272	LEU	N-CA-C	5.07	124.70	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	TYR	Sidechain
1	C	131	TYR	Sidechain

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	1232	0	1218	105	0
1	B	1232	0	1218	110	0
1	C	1232	0	1218	110	0
All	All	3696	0	3654	325	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 44.

All (325) 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:C:218:LEU:HD22	1:C:222:ILE:HD12	1.43	0.98
1:B:218:LEU:HD22	1:B:222:ILE:HD12	1.44	0.97
1:A:218:LEU:HD22	1:A:222:ILE:HD12	1.45	0.97
1:B:212:ASN:HD22	1:B:289:ALA:HB2	1.40	0.86
1:C:212:ASN:HD22	1:C:289:ALA:HB2	1.41	0.86
1:A:226:GLN:O	1:A:230:ILE:HG13	1.77	0.85
1:C:226:GLN:O	1:C:230:ILE:HG13	1.76	0.84
1:B:243:LEU:HD13	1:B:255:ALA:HA	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:N	1:B:274:ASN:HD22	1.76	0.83
1:B:226:GLN:O	1:B:230:ILE:HG13	1.79	0.83
1:C:218:LEU:HD22	1:C:222:ILE:CD1	2.08	0.83
1:A:218:LEU:HD22	1:A:222:ILE:CD1	2.09	0.82
1:C:243:LEU:HD13	1:C:255:ALA:HA	1.62	0.81
1:A:243:LEU:HD13	1:A:255:ALA:HA	1.62	0.81
1:A:187:ASN:HD22	1:A:198:VAL:N	1.78	0.81
1:C:274:ASN:N	1:C:274:ASN:HD22	1.79	0.81
1:A:234:TYR:O	1:A:264:GLU:HB3	1.82	0.80
1:B:218:LEU:HD22	1:B:222:ILE:CD1	2.11	0.80
1:A:274:ASN:N	1:A:274:ASN:HD22	1.80	0.79
1:B:234:TYR:O	1:B:264:GLU:HB3	1.83	0.78
1:B:187:ASN:HD22	1:B:198:VAL:N	1.81	0.78
1:C:187:ASN:HD22	1:C:198:VAL:N	1.83	0.77
1:C:234:TYR:O	1:C:264:GLU:HB3	1.84	0.77
1:A:206:GLU:N	1:A:209:LYS:HB2	2.00	0.75
1:C:232:GLY:N	1:C:237:ILE:HD11	2.01	0.75
1:C:206:GLU:N	1:C:209:LYS:HB2	2.02	0.74
1:A:187:ASN:HD22	1:A:198:VAL:H	1.32	0.74
1:B:137:THR:CG2	1:B:139:ARG:HB2	2.18	0.74
1:B:283:PRO:O	1:B:284:LEU:HB2	1.86	0.74
1:A:244:ARG:HA	1:A:251:PRO:HA	1.70	0.74
1:B:232:GLY:N	1:B:237:ILE:HD11	2.02	0.74
1:A:222:ILE:HA	1:A:226:GLN:NE2	2.02	0.74
1:B:181:ARG:O	1:B:185:VAL:HG23	1.88	0.74
1:B:187:ASN:HD22	1:B:198:VAL:H	1.36	0.74
1:B:206:GLU:N	1:B:209:LYS:HB2	2.03	0.73
1:A:187:ASN:ND2	1:A:198:VAL:H	1.85	0.73
1:C:181:ARG:O	1:C:185:VAL:HG23	1.89	0.73
1:C:222:ILE:HA	1:C:226:GLN:NE2	2.03	0.73
1:A:232:GLY:N	1:A:237:ILE:HD11	2.03	0.73
1:A:211:THR:HG22	1:A:211:THR:O	1.89	0.73
1:B:222:ILE:HA	1:B:226:GLN:NE2	2.03	0.73
1:B:244:ARG:HA	1:B:251:PRO:HA	1.71	0.73
1:B:211:THR:HG22	1:B:211:THR:O	1.89	0.72
1:C:283:PRO:O	1:C:284:LEU:HB2	1.89	0.72
1:C:244:ARG:HA	1:C:251:PRO:HA	1.71	0.72
1:A:181:ARG:O	1:A:185:VAL:HG23	1.90	0.72
1:A:212:ASN:HD22	1:A:289:ALA:HB2	1.54	0.72
1:B:187:ASN:ND2	1:B:198:VAL:H	1.87	0.72
1:A:137:THR:CG2	1:A:139:ARG:HB2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:THR:O	1:C:211:THR:HG22	1.88	0.71
1:A:222:ILE:HA	1:A:226:GLN:HE22	1.56	0.70
1:C:137:THR:CG2	1:C:139:ARG:HB2	2.21	0.70
1:B:212:ASN:ND2	1:B:289:ALA:HB2	2.05	0.70
1:B:222:ILE:HA	1:B:226:GLN:HE22	1.57	0.70
1:C:222:ILE:HA	1:C:226:GLN:HE22	1.56	0.69
1:B:274:ASN:N	1:B:274:ASN:ND2	2.39	0.69
1:A:283:PRO:O	1:A:284:LEU:HB2	1.90	0.69
1:C:177[B]:MSE:O	1:C:181:ARG:HG3	1.92	0.69
1:B:187:ASN:ND2	1:B:198:VAL:N	2.41	0.68
1:A:177[A]:MSE:O	1:A:181:ARG:HG3	1.92	0.68
1:C:187:ASN:HD22	1:C:198:VAL:H	1.41	0.68
1:C:212:ASN:ND2	1:C:289:ALA:HB2	2.08	0.68
1:A:187:ASN:ND2	1:A:198:VAL:N	2.39	0.68
1:A:288:LEU:N	1:A:288:LEU:HD22	2.09	0.68
1:C:187:ASN:ND2	1:C:198:VAL:N	2.43	0.67
1:C:288:LEU:HD22	1:C:288:LEU:N	2.09	0.67
1:B:177[B]:MSE:O	1:B:181:ARG:HG3	1.93	0.67
1:B:288:LEU:N	1:B:288:LEU:HD22	2.09	0.67
1:B:137:THR:HG22	1:B:139:ARG:HB2	1.75	0.67
1:C:137:THR:HG22	1:C:139:ARG:H	1.60	0.67
1:C:187:ASN:ND2	1:C:198:VAL:H	1.92	0.67
1:B:132:LEU:HD23	1:B:196:LEU:HD21	1.77	0.67
1:A:137:THR:HG22	1:A:139:ARG:HB2	1.77	0.66
1:C:274:ASN:N	1:C:274:ASN:ND2	2.42	0.66
1:A:137:THR:HG22	1:A:139:ARG:H	1.61	0.66
1:C:132:LEU:HD23	1:C:196:LEU:HD21	1.76	0.66
1:A:274:ASN:N	1:A:274:ASN:ND2	2.42	0.65
1:A:132:LEU:HD23	1:A:196:LEU:HD21	1.79	0.65
1:C:137:THR:HG22	1:C:139:ARG:HB2	1.79	0.65
1:B:215:VAL:HG12	1:B:286:VAL:HG12	1.79	0.65
1:C:218:LEU:CD2	1:C:222:ILE:HD12	2.23	0.64
1:C:206:GLU:CA	1:C:209:LYS:HB2	2.27	0.64
1:B:206:GLU:CA	1:B:209:LYS:HB2	2.27	0.64
1:A:206:GLU:CA	1:A:209:LYS:HB2	2.27	0.64
1:C:140:GLU:OE2	1:C:192:ARG:NH2	2.29	0.64
1:A:238:VAL:O	1:A:239:GLN:HB3	1.98	0.63
1:B:218:LEU:CD2	1:B:222:ILE:HD12	2.24	0.63
1:C:274:ASN:O	1:C:275:VAL:C	2.36	0.63
1:A:137:THR:HG22	1:A:139:ARG:N	2.14	0.62
1:A:140:GLU:OE2	1:A:192:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HG12	1:A:286:VAL:HG12	1.81	0.62
1:B:274:ASN:O	1:B:275:VAL:C	2.37	0.62
1:C:243:LEU:HD12	1:C:243:LEU:N	2.14	0.62
1:A:274:ASN:O	1:A:275:VAL:C	2.38	0.62
1:C:137:THR:HG22	1:C:139:ARG:N	2.14	0.62
1:A:157:MSE:HA	1:A:157:MSE:HE3	1.81	0.62
1:C:215:VAL:HG12	1:C:286:VAL:HG12	1.81	0.62
1:C:238:VAL:O	1:C:239:GLN:HB3	1.99	0.61
1:B:157:MSE:HE3	1:B:157:MSE:HA	1.83	0.61
1:B:243:LEU:N	1:B:243:LEU:HD12	2.15	0.61
1:C:187:ASN:HD21	1:C:197:LYS:HG3	1.66	0.61
1:B:140:GLU:OE2	1:B:192:ARG:NH2	2.34	0.61
1:B:238:VAL:O	1:B:239:GLN:HB3	2.01	0.61
1:A:238:VAL:HG22	1:A:258:ARG:O	2.01	0.61
1:A:127:LEU:HD13	1:A:198:VAL:CG1	2.30	0.60
1:B:137:THR:HG22	1:B:139:ARG:H	1.66	0.60
1:A:243:LEU:N	1:A:243:LEU:HD12	2.15	0.60
1:C:269:ILE:O	1:C:273:ASN:ND2	2.33	0.60
1:A:187:ASN:HD21	1:A:197:LYS:HG3	1.67	0.60
1:B:127:LEU:HD13	1:B:198:VAL:CG1	2.33	0.59
1:C:238:VAL:HG22	1:C:258:ARG:O	2.02	0.59
1:A:207:SER:C	1:A:211:THR:HB	2.23	0.59
1:B:137:THR:HG22	1:B:139:ARG:N	2.17	0.59
1:B:187:ASN:HD21	1:B:197:LYS:HG3	1.67	0.59
1:C:177[A]:MSE:O	1:C:181:ARG:HG3	2.02	0.59
1:C:157:MSE:HE3	1:C:157:MSE:HA	1.85	0.59
1:A:212:ASN:ND2	1:A:289:ALA:HB2	2.18	0.58
1:C:127:LEU:HD13	1:C:198:VAL:CG1	2.33	0.58
1:C:243:LEU:N	1:C:243:LEU:CD1	2.66	0.58
1:C:207:SER:C	1:C:211:THR:HB	2.23	0.58
1:A:177[B]:MSE:O	1:A:181:ARG:HG3	2.04	0.58
1:B:211:THR:CG2	1:B:259:TYR:O	2.52	0.58
1:B:142:TYR:HE1	1:B:151:ILE:HB	1.70	0.57
1:B:243:LEU:N	1:B:243:LEU:CD1	2.66	0.57
1:A:243:LEU:N	1:A:243:LEU:CD1	2.67	0.57
1:A:269:ILE:O	1:A:273:ASN:ND2	2.36	0.57
1:C:133:PRO:HG2	1:C:136:MSE:HB2	1.87	0.57
1:A:211:THR:CG2	1:A:259:TYR:O	2.53	0.56
1:C:211:THR:CG2	1:C:259:TYR:O	2.54	0.56
1:B:238:VAL:HG22	1:B:258:ARG:O	2.05	0.56
1:A:218:LEU:CD2	1:A:222:ILE:HD12	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:CG2	1:A:139:ARG:H	2.19	0.56
1:B:269:ILE:O	1:B:273:ASN:ND2	2.38	0.56
1:C:137:THR:CG2	1:C:139:ARG:H	2.18	0.56
1:C:206:GLU:O	1:C:210:ASP:N	2.39	0.56
1:B:133:PRO:HG2	1:B:136:MSE:HB2	1.87	0.55
1:B:207:SER:C	1:B:211:THR:HB	2.26	0.55
1:C:142:TYR:HE1	1:C:151:ILE:HB	1.71	0.55
1:A:288:LEU:N	1:A:288:LEU:CD2	2.69	0.55
1:B:206:GLU:O	1:B:210:ASP:N	2.38	0.55
1:A:142:TYR:HE1	1:A:151:ILE:HB	1.70	0.55
1:A:206:GLU:O	1:A:210:ASP:N	2.39	0.55
1:C:288:LEU:N	1:C:288:LEU:CD2	2.69	0.55
1:B:137:THR:HG22	1:B:140:GLU:H	1.72	0.55
1:C:218:LEU:HB2	1:C:253:GLY:O	2.07	0.55
1:A:133:PRO:HG2	1:A:136:MSE:HB2	1.88	0.55
1:B:177[A]:MSE:O	1:B:181:ARG:HG3	2.05	0.55
1:C:148:ILE:N	1:C:148:ILE:HD12	2.23	0.54
1:B:288:LEU:N	1:B:288:LEU:CD2	2.70	0.54
1:A:162:THR:HG21	1:A:164:TYR:HB2	1.89	0.54
1:A:223:THR:H	1:A:226:GLN:HE21	1.56	0.54
1:B:162:THR:HG21	1:B:164:TYR:HB2	1.89	0.54
1:B:128:ILE:HD11	1:B:201:ALA:HA	1.89	0.54
1:B:148:ILE:N	1:B:148:ILE:HD12	2.24	0.53
1:B:283:PRO:O	1:B:284:LEU:CB	2.56	0.53
1:A:206:GLU:HA	1:A:209:LYS:HB2	1.91	0.53
1:C:206:GLU:HA	1:C:209:LYS:HB2	1.91	0.53
1:A:227:LEU:O	1:A:231:PHE:HD1	1.92	0.53
1:B:218:LEU:HB2	1:B:253:GLY:O	2.08	0.53
1:C:128:ILE:HD11	1:C:201:ALA:HA	1.91	0.53
1:B:137:THR:CG2	1:B:139:ARG:H	2.21	0.53
1:A:133:PRO:HA	1:A:194:LYS:HG3	1.91	0.53
1:A:138:ASP:OD1	1:A:156:ILE:HB	2.09	0.52
1:A:223:THR:H	1:A:226:GLN:NE2	2.07	0.52
1:B:223:THR:H	1:B:226:GLN:HE21	1.57	0.52
1:C:223:THR:H	1:C:226:GLN:HE21	1.57	0.52
1:B:206:GLU:HA	1:B:209:LYS:HB2	1.91	0.52
1:C:162:THR:HG21	1:C:164:TYR:HB2	1.91	0.52
1:A:218:LEU:HB2	1:A:253:GLY:O	2.09	0.52
1:C:223:THR:H	1:C:226:GLN:NE2	2.08	0.52
1:A:148:ILE:HD12	1:A:148:ILE:N	2.25	0.52
1:C:238:VAL:O	1:C:239:GLN:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASN:ND2	1:B:283:PRO:HB2	2.24	0.52
1:A:238:VAL:O	1:A:239:GLN:CB	2.57	0.51
1:B:223:THR:H	1:B:226:GLN:NE2	2.08	0.51
1:B:227:LEU:O	1:B:231:PHE:HD1	1.93	0.51
1:C:137:THR:HG22	1:C:140:GLU:H	1.75	0.51
1:B:133:PRO:HA	1:B:194:LYS:HG3	1.92	0.51
1:C:133:PRO:HA	1:C:194:LYS:HG3	1.92	0.51
1:C:283:PRO:O	1:C:284:LEU:CB	2.58	0.51
1:C:138:ASP:OD1	1:C:156:ILE:HB	2.10	0.51
1:C:244:ARG:NH1	1:C:251:PRO:HG3	2.26	0.50
1:B:138:ASP:OD1	1:B:156:ILE:HB	2.12	0.50
1:A:137:THR:HG22	1:A:140:GLU:H	1.75	0.50
1:B:232:GLY:CA	1:B:237:ILE:HD11	2.41	0.50
1:C:217:ASN:ND2	1:C:283:PRO:HB2	2.25	0.50
1:C:214:TYR:CD1	1:C:256:PHE:CZ	2.99	0.50
1:C:227:LEU:O	1:C:231:PHE:HD1	1.95	0.50
1:A:128:ILE:HD11	1:A:201:ALA:HA	1.94	0.50
1:B:231:PHE:CE2	1:B:257:VAL:HG11	2.47	0.50
1:A:159:ASP:HB3	1:A:162:THR:HB	1.95	0.49
1:B:159:ASP:HB3	1:B:162:THR:HB	1.95	0.49
1:A:137:THR:HG21	1:A:139:ARG:HB2	1.95	0.49
1:B:192:ARG:O	1:B:193:ASN:HB2	2.13	0.49
1:C:232:GLY:CA	1:C:237:ILE:HD11	2.42	0.49
1:C:231:PHE:CE2	1:C:257:VAL:HG11	2.48	0.49
1:C:159:ASP:HB3	1:C:162:THR:HB	1.95	0.49
1:C:269:ILE:HA	1:C:286:VAL:HG21	1.94	0.49
1:A:220:ARG:HD3	1:A:252:ARG:HA	1.95	0.49
1:A:238:VAL:HG23	1:A:239:GLN:HG2	1.94	0.49
1:A:257:VAL:HG13	1:A:257:VAL:O	2.13	0.48
1:A:207:SER:O	1:A:211:THR:HB	2.13	0.48
1:A:214:TYR:CD1	1:A:256:PHE:CZ	3.01	0.48
1:A:217:ASN:ND2	1:A:283:PRO:HB2	2.29	0.48
1:B:142:TYR:CE1	1:B:151:ILE:HD12	2.48	0.48
1:B:220:ARG:HD3	1:B:252:ARG:HA	1.96	0.48
1:A:211:THR:O	1:A:211:THR:CG2	2.60	0.48
1:A:219:PRO:C	1:A:221:THR:H	2.17	0.48
1:A:232:GLY:CA	1:A:237:ILE:HD11	2.43	0.48
1:C:207:SER:O	1:C:211:THR:HB	2.14	0.48
1:A:192:ARG:O	1:A:193:ASN:HB2	2.14	0.47
1:A:231:PHE:CE2	1:A:257:VAL:HG11	2.50	0.47
1:A:244:ARG:NH1	1:A:251:PRO:HG3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:VAL:HG23	1:C:239:GLN:HG2	1.96	0.47
1:A:208:ILE:O	1:A:209:LYS:HD3	2.14	0.47
1:B:257:VAL:HG13	1:B:257:VAL:O	2.13	0.47
1:C:142:TYR:CE1	1:C:151:ILE:HD12	2.49	0.47
1:A:259:TYR:CD2	1:A:265:ALA:HA	2.49	0.47
1:B:219:PRO:C	1:B:221:THR:H	2.18	0.47
1:B:238:VAL:O	1:B:239:GLN:CB	2.60	0.47
1:B:259:TYR:CD2	1:B:265:ALA:HA	2.49	0.47
1:C:159:ASP:HB3	1:C:163:GLY:H	1.79	0.47
1:C:219:PRO:C	1:C:221:THR:H	2.17	0.47
1:A:142:TYR:CE1	1:A:151:ILE:HD12	2.50	0.47
1:A:275:VAL:HB	1:A:283:PRO:N	2.29	0.47
1:B:211:THR:O	1:B:211:THR:CG2	2.61	0.47
1:C:211:THR:O	1:C:211:THR:CG2	2.60	0.47
1:C:257:VAL:HG13	1:C:257:VAL:O	2.14	0.47
1:C:269:ILE:HG23	1:C:273:ASN:HD21	1.80	0.47
1:B:137:THR:HG21	1:B:139:ARG:HB2	1.94	0.47
1:B:214:TYR:CD1	1:B:256:PHE:CZ	3.03	0.47
1:C:259:TYR:CD2	1:C:265:ALA:HA	2.49	0.47
1:B:244:ARG:NH1	1:B:251:PRO:HG3	2.30	0.47
1:B:146:ARG:HA	1:B:146:ARG:HD2	1.42	0.46
1:A:214:TYR:N	1:A:287:ARG:O	2.38	0.46
1:B:269:ILE:HG23	1:B:273:ASN:HD21	1.80	0.46
1:B:269:ILE:HA	1:B:286:VAL:HG21	1.98	0.46
1:B:207:SER:O	1:B:211:THR:HB	2.15	0.46
1:A:216:THR:HG22	1:A:254:VAL:HG12	1.98	0.46
1:B:159:ASP:HB3	1:B:163:GLY:H	1.80	0.46
1:C:137:THR:HG21	1:C:139:ARG:HB2	1.96	0.46
1:A:248:THR:HG22	1:A:250:ARG:H	1.81	0.46
1:C:141:LEU:HD11	1:C:145:PHE:HE1	1.81	0.46
1:C:214:TYR:N	1:C:287:ARG:O	2.40	0.46
1:C:220:ARG:HD3	1:C:252:ARG:HA	1.97	0.46
1:A:269:ILE:HG23	1:A:273:ASN:HD21	1.81	0.45
1:C:240:LYS:HD2	1:C:240:LYS:O	2.16	0.45
1:B:238:VAL:HG23	1:B:239:GLN:HG2	1.98	0.45
1:B:214:TYR:N	1:B:287:ARG:O	2.36	0.45
1:B:240:LYS:HD2	1:B:240:LYS:O	2.16	0.45
1:C:215:VAL:HG22	1:C:255:ALA:O	2.17	0.45
1:C:248:THR:HG22	1:C:250:ARG:H	1.82	0.45
1:A:283:PRO:O	1:A:284:LEU:CB	2.60	0.45
1:C:269:ILE:HA	1:C:286:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HG12	1:B:198:VAL:HG12	1.98	0.45
1:C:127:LEU:HD13	1:C:198:VAL:HG13	1.99	0.45
1:B:213:LEU:HA	1:B:287:ARG:O	2.17	0.45
1:A:159:ASP:HB3	1:A:163:GLY:H	1.82	0.44
1:B:127:LEU:HD13	1:B:198:VAL:HG13	1.99	0.44
1:C:146:ARG:HD2	1:C:146:ARG:HA	1.42	0.44
1:C:192:ARG:O	1:C:193:ASN:HB2	2.17	0.44
1:B:208:ILE:O	1:B:209:LYS:HD3	2.17	0.44
1:C:201:ALA:O	1:C:203:PRO:HD3	2.18	0.44
1:B:269:ILE:HA	1:B:286:VAL:CG2	2.47	0.44
1:B:248:THR:O	1:B:248:THR:HG22	2.17	0.44
1:A:269:ILE:HA	1:A:286:VAL:HG21	1.98	0.43
1:A:215:VAL:HG22	1:A:255:ALA:O	2.18	0.43
1:A:245:ASP:O	1:A:249:GLY:N	2.49	0.43
1:B:217:ASN:HD21	1:B:283:PRO:HB2	1.83	0.43
1:A:124:ASN:N	1:A:176:GLU:OE1	2.51	0.43
1:C:243:LEU:CD1	1:C:243:LEU:H	2.31	0.43
1:A:240:LYS:HD2	1:A:240:LYS:O	2.19	0.43
1:C:159:ASP:O	1:C:163:GLY:HA2	2.18	0.43
1:A:127:LEU:HD13	1:A:198:VAL:HG13	1.98	0.43
1:A:201:ALA:O	1:A:203:PRO:HD3	2.18	0.43
1:C:208:ILE:O	1:C:209:LYS:HD3	2.18	0.43
1:C:183:ILE:HG12	1:C:198:VAL:HG12	2.00	0.43
1:B:243:LEU:CD1	1:B:243:LEU:H	2.31	0.42
1:A:243:LEU:CD1	1:A:243:LEU:H	2.32	0.42
1:B:216:THR:HG22	1:B:254:VAL:HG12	2.02	0.42
1:B:218:LEU:CD2	1:B:222:ILE:CD1	2.92	0.42
1:A:226:GLN:O	1:A:230:ILE:CG1	2.60	0.42
1:B:248:THR:HG22	1:B:250:ARG:H	1.84	0.42
1:B:159:ASP:O	1:B:163:GLY:HA2	2.19	0.42
1:B:244:ARG:HG2	1:B:251:PRO:HG3	2.00	0.42
1:C:218:LEU:HB2	1:C:253:GLY:C	2.40	0.42
1:C:288:LEU:O	1:C:289:ALA:C	2.57	0.42
1:B:215:VAL:HG22	1:B:255:ALA:O	2.20	0.42
1:B:288:LEU:CD2	1:B:288:LEU:H	2.33	0.42
1:A:183:ILE:HG12	1:A:198:VAL:HG12	2.01	0.42
1:B:141:LEU:HD11	1:B:145:PHE:HE1	1.85	0.42
1:B:275:VAL:HB	1:B:283:PRO:N	2.35	0.42
1:C:141:LEU:HD11	1:C:145:PHE:CE1	2.54	0.42
1:C:248:THR:HG22	1:C:248:THR:O	2.18	0.42
1:A:269:ILE:HA	1:A:286:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HD23	1:C:196:LEU:HA	1.78	0.42
1:C:288:LEU:CD2	1:C:288:LEU:H	2.33	0.42
1:A:261:LYS:C	1:A:263:GLU:N	2.73	0.41
1:B:124:ASN:N	1:B:176:GLU:OE1	2.53	0.41
1:B:288:LEU:O	1:B:289:ALA:C	2.58	0.41
1:C:124:ASN:N	1:C:176:GLU:OE1	2.53	0.41
1:C:275:VAL:HB	1:C:283:PRO:N	2.35	0.41
1:A:141:LEU:HD11	1:A:145:PHE:HE1	1.84	0.41
1:A:248:THR:HG22	1:A:248:THR:O	2.18	0.41
1:B:139:ARG:HG3	1:B:139:ARG:NH1	2.35	0.41
1:B:201:ALA:O	1:B:203:PRO:HD3	2.19	0.41
1:C:227:LEU:HD12	1:C:227:LEU:HA	1.87	0.41
1:C:245:ASP:O	1:C:249:GLY:N	2.52	0.41
1:B:142:TYR:CD1	1:B:151:ILE:HD12	2.56	0.41
1:A:157:MSE:HA	1:A:157:MSE:CE	2.49	0.41
1:B:130:ASN:O	1:B:196:LEU:HD23	2.19	0.41
1:C:216:THR:HG22	1:C:254:VAL:HG12	2.02	0.41
1:C:244:ARG:HG2	1:C:251:PRO:HG3	2.01	0.41
1:A:159:ASP:O	1:A:163:GLY:HA2	2.21	0.41
1:B:261:LYS:C	1:B:263:GLU:N	2.72	0.41
1:C:217:ASN:HD21	1:C:283:PRO:HB2	1.86	0.41
1:B:148:ILE:N	1:B:148:ILE:CD1	2.84	0.40
1:B:218:LEU:HB2	1:B:253:GLY:C	2.41	0.40
1:A:218:LEU:HB2	1:A:253:GLY:C	2.42	0.40
1:C:148:ILE:N	1:C:148:ILE:CD1	2.84	0.40
1:C:261:LYS:C	1:C:263:GLU:N	2.72	0.40
1:A:130:ASN:O	1:A:196:LEU:HD23	2.20	0.40
1:A:139:ARG:NH1	1:A:139:ARG:HG3	2.36	0.40
1:A:148:ILE:N	1:A:148:ILE:CD1	2.84	0.40
1:C:213:LEU:HA	1:C:287:ARG:O	2.22	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	152/184 (83%)	135 (89%)	15 (10%)	2 (1%)	12	30
1	B	152/184 (83%)	135 (89%)	15 (10%)	2 (1%)	12	30
1	C	152/184 (83%)	136 (90%)	14 (9%)	2 (1%)	12	30
All	All	456/552 (83%)	406 (89%)	44 (10%)	6 (1%)	12	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	284	LEU
1	B	284	LEU
1	C	284	LEU
1	B	239	GLN
1	C	239	GLN

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	131/156 (84%)	115 (88%)	16 (12%)	5	11
1	B	131/156 (84%)	114 (87%)	17 (13%)	4	10
1	C	131/156 (84%)	115 (88%)	16 (12%)	5	11
All	All	393/468 (84%)	344 (88%)	49 (12%)	4	10

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	126	ASN
1	A	144	LEU
1	A	146	ARG

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Mol	Chain	Res	Type
1	A	154	CYS
1	A	157	MSE
1	A	191	VAL
1	A	195	ARG
1	A	206	GLU
1	A	210	ASP
1	A	240	LYS
1	A	247	LEU
1	A	266	GLN
1	A	274	ASN
1	A	284	LEU
1	A	288	LEU
1	B	124	ASN
1	B	126	ASN
1	B	144	LEU
1	B	146	ARG
1	B	154	CYS
1	B	157	MSE
1	B	191	VAL
1	B	195	ARG
1	B	206	GLU
1	B	210	ASP
1	B	213	LEU
1	B	240	LYS
1	B	247	LEU
1	B	266	GLN
1	B	274	ASN
1	B	284	LEU
1	B	288	LEU
1	C	124	ASN
1	C	126	ASN
1	C	144	LEU
1	C	146	ARG
1	C	154	CYS
1	C	157	MSE
1	C	191	VAL
1	C	195	ARG
1	C	206	GLU
1	C	210	ASP
1	C	240	LYS
1	C	247	LEU
1	C	266	GLN

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Mol	Chain	Res	Type
1	C	274	ASN
1	C	284	LEU
1	C	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	212	ASN
1	A	217	ASN
1	A	226	GLN
1	A	266	GLN
1	A	274	ASN
1	B	187	ASN
1	B	212	ASN
1	B	217	ASN
1	B	226	GLN
1	B	266	GLN
1	B	274	ASN
1	C	187	ASN
1	C	212	ASN
1	C	217	ASN
1	C	226	GLN
1	C	266	GLN
1	C	274	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	154/184 (83%)	-0.33	1 (0%) 89 91	28, 57, 79, 96	0
1	B	154/184 (83%)	-0.29	0 100 100	28, 58, 79, 96	0
1	C	154/184 (83%)	-0.33	0 100 100	28, 57, 79, 96	0
All	All	462/552 (83%)	-0.32	1 (0%) 95 96	28, 58, 79, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	VAL	2.2

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.