



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:13 am BST

PDB ID : 6N9O
Title : Crystal structure of human GSDMD
Authors : Liu, Z.; Wang, C.; Yang, J.; Xiao, T.S.
Deposited on : 2018-12-03
Resolution : 3.50 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 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	:	2.11
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)	:	2.11

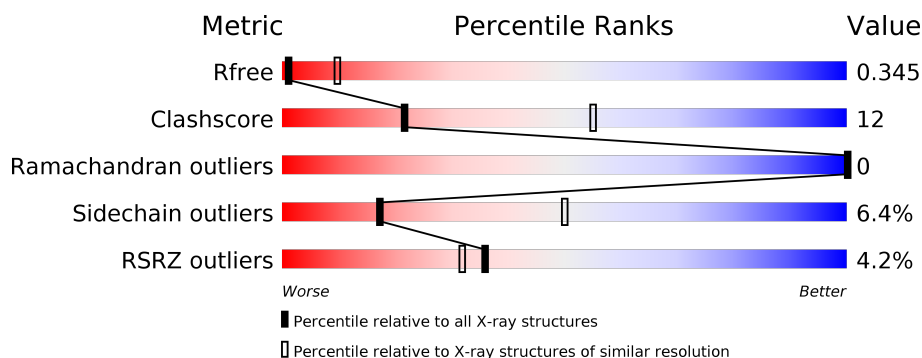
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	485	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>20%</div> <div>•</div> <div>24%</div> </div> </div>
1	B	485	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>23%</div> <div>•</div> <div>24%</div> </div> </div>
1	C	485	<div> <div>0%</div> <div> <div></div> <div>55%</div> <div>22%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	485	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>21%</div> <div>•</div> <div>22%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11601 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 Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2879	1825	481	560	13			
1	B	369	Total	C	N	O	S	0	0	0
			2871	1822	480	556	13			
1	C	379	Total	C	N	O	S	0	0	0
			2930	1860	490	566	14			
1	D	377	Total	C	N	O	S	0	0	0
			2921	1854	487	567	13			

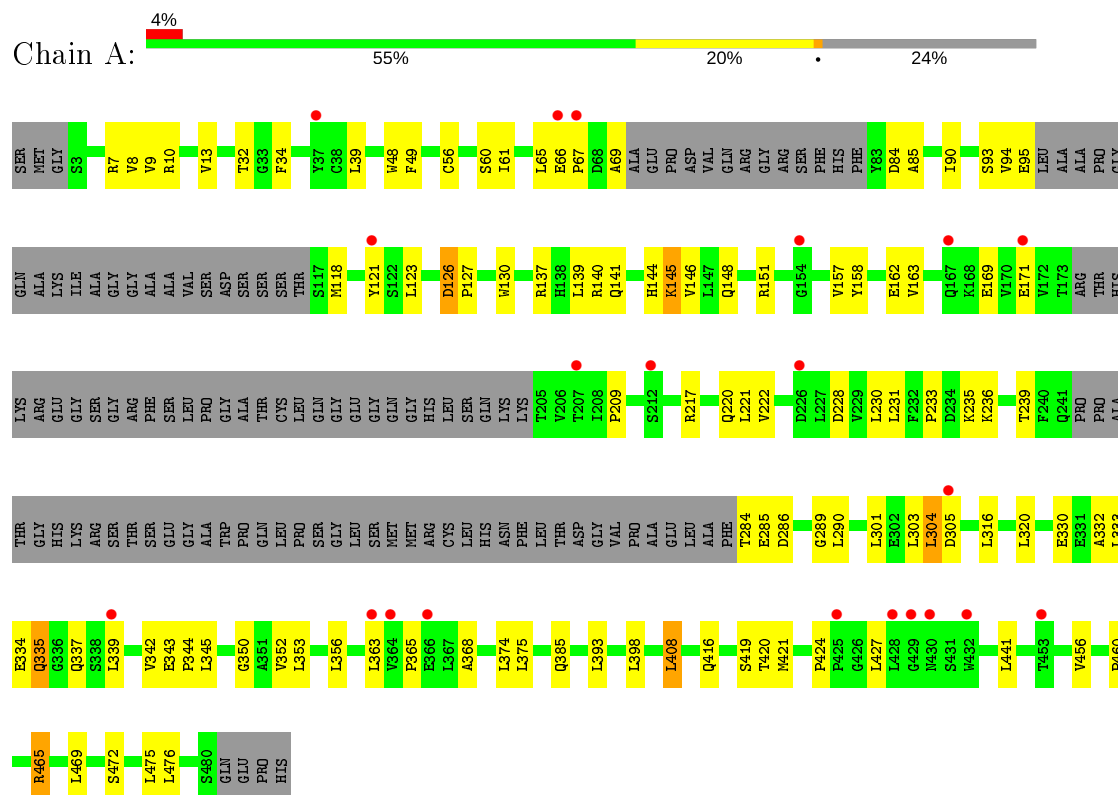
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P57764
A	281	LEU	GLY	conflict	UNP P57764
B	0	SER	-	expression tag	UNP P57764
B	281	LEU	GLY	conflict	UNP P57764
C	0	SER	-	expression tag	UNP P57764
C	281	LEU	GLY	conflict	UNP P57764
D	0	SER	-	expression tag	UNP P57764
D	281	LEU	GLY	conflict	UNP P57764

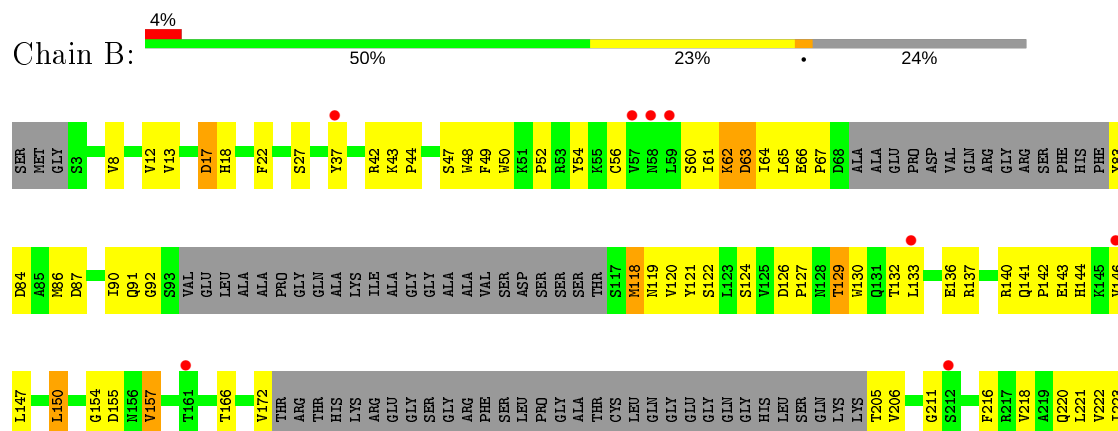
3 Residue-property plots [i](#)

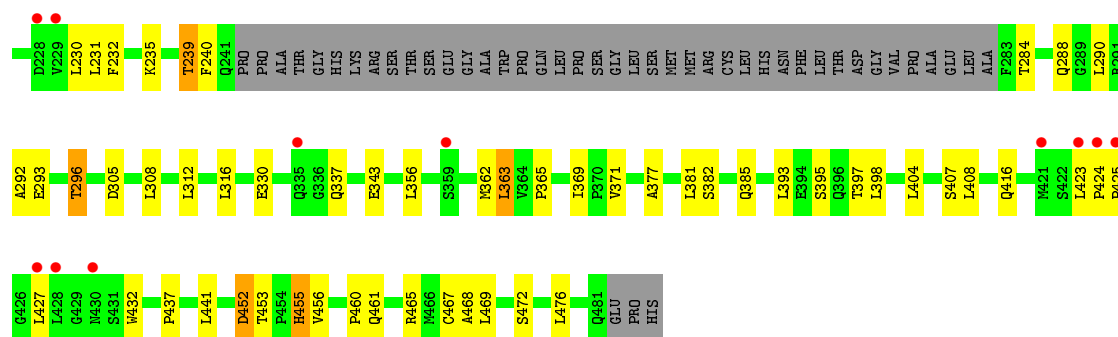
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Gasdermin-D

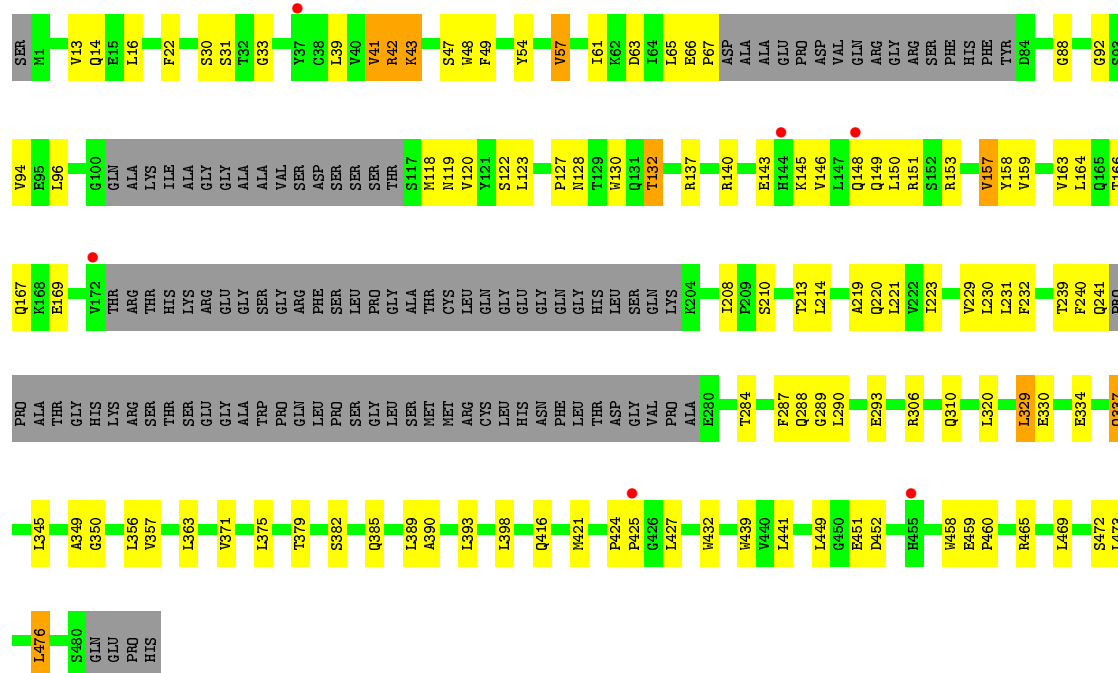


• Molecule 1: Gasdermin-D

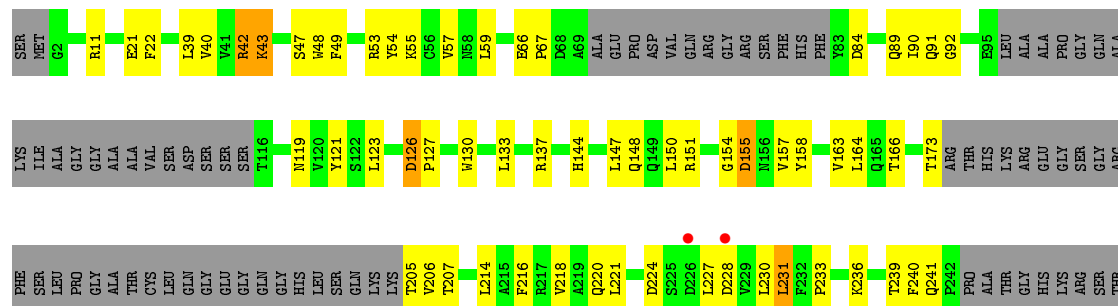


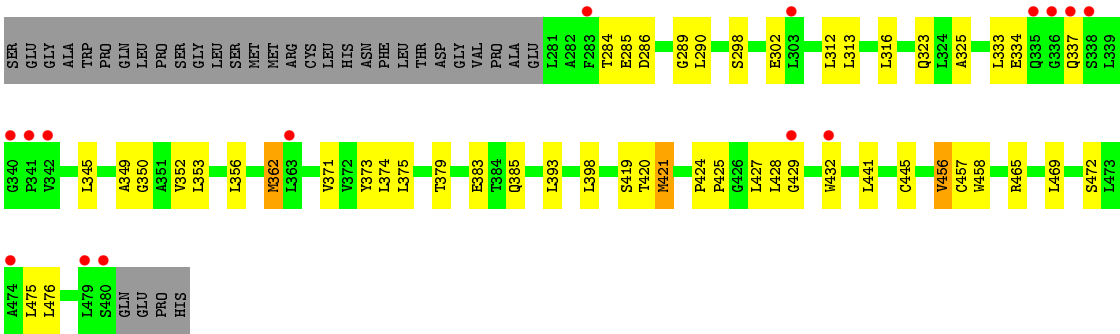


• Molecule 1: Gasdermin-D



• Molecule 1: Gasdermin-D





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.64Å 105.55Å 151.79Å 90.00° 94.47° 90.00°	Depositor
Resolution (Å)	49.48 – 3.50 49.48 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.48-3.50) 99.2 (49.48-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.276 , 0.345 0.277 , 0.345	Depositor DCC
R_{free} test set	1116 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	153.7	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 124.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11601	wwPDB-VP
Average B, all atoms (Å ²)	182.0	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.*

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	0.28	0/2930	0.54	0/3983
1	B	0.29	0/2923	0.56	0/3972
1	C	0.28	0/2982	0.52	0/4051
1	D	0.28	0/2974	0.51	0/4044
All	All	0.28	0/11809	0.53	0/16050

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	2879	0	2879	66	0
1	B	2871	0	2869	77	0
1	C	2930	0	2944	68	0
1	D	2921	0	2921	71	0
All	All	11601	0	11613	276	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 12.

All (276) 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:D:157:VAL:H	1:D:239:THR:HG21	1.30	0.94
1:D:47:SER:HB2	1:D:373:TYR:HE1	1.37	0.89
1:D:53:ARG:HH21	1:D:379:THR:HB	1.40	0.84
1:B:67:PRO:HD3	1:B:137:ARG:HG2	1.60	0.82
1:D:166:THR:HG23	1:D:214:LEU:HD11	1.66	0.76
1:D:323:GLN:HE21	1:D:383:GLU:HG3	1.51	0.76
1:C:153:ARG:HA	1:C:337:GLN:HG2	1.65	0.75
1:D:126:ASP:N	1:D:126:ASP:OD1	2.20	0.75
1:A:286:ASP:O	1:A:289:GLY:N	2.21	0.73
1:A:145:LYS:HD2	1:A:146:VAL:HG13	1.69	0.73
1:C:92:GLY:HA2	1:C:119:ASN:HA	1.70	0.71
1:C:39:LEU:HG	1:C:159:VAL:HG12	1.70	0.71
1:A:421:MET:HB2	1:A:456:VAL:HG11	1.71	0.70
1:D:421:MET:HB2	1:D:456:VAL:HG13	1.74	0.69
1:C:167:GLN:HG3	1:C:210:SER:HB2	1.72	0.69
1:C:424:PRO:HG2	1:C:427:LEU:HB2	1.74	0.69
1:D:323:GLN:NE2	1:D:383:GLU:HG3	2.07	0.69
1:D:66:GLU:HB3	1:D:67:PRO:HD3	1.75	0.68
1:B:221:LEU:O	1:B:239:THR:HG23	1.94	0.68
1:D:49:PHE:HE2	1:D:290:LEU:HB2	1.59	0.68
1:D:144:HIS:HB3	1:D:148:GLN:HB2	1.77	0.67
1:A:90:ILE:HG12	1:A:121:TYR:HE1	1.60	0.67
1:B:87:ASP:HB2	1:B:124:SER:HB2	1.77	0.67
1:A:416:GLN:HA	1:A:460:PRO:HB3	1.77	0.67
1:C:96:LEU:HD11	1:C:118:MET:HB3	1.77	0.67
1:D:445:CYS:HA	1:D:465:ARG:HD2	1.78	0.66
1:B:127:PRO:HA	1:B:130:TRP:HD1	1.60	0.66
1:D:325:ALA:HB1	1:D:349:ALA:HB2	1.78	0.65
1:D:333:LEU:HD11	1:D:353:LEU:HD13	1.78	0.64
1:C:43:LYS:NZ	1:C:330:GLU:OE2	2.24	0.64
1:D:47:SER:HB2	1:D:373:TYR:CE1	2.26	0.64
1:B:136:GLU:OE1	1:B:137:ARG:NH2	2.30	0.64
1:D:148:GLN:HA	1:D:151:ARG:HG2	1.78	0.64
1:A:39:LEU:HD11	1:A:61:ILE:HB	1.79	0.63
1:B:86:MET:HG2	1:B:87:ASP:H	1.63	0.63
1:A:304:LEU:HD13	1:A:305:ASP:H	1.62	0.63
1:B:66:GLU:N	1:B:67:PRO:HD2	2.13	0.63
1:A:344:PRO:HA	1:A:353:LEU:HD23	1.81	0.63
1:B:381:LEU:HD21	1:B:469:LEU:HB2	1.79	0.63
1:B:65:LEU:HB3	1:B:67:PRO:HD2	1.82	0.62
1:A:90:ILE:HG12	1:A:121:TYR:CE1	2.35	0.62
1:A:162:GLU:OE1	1:A:217:ARG:NH1	2.23	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:PRO:HA	1:D:130:TRP:HD1	1.65	0.61
1:B:290:LEU:HD21	1:B:467:CYS:HB3	1.82	0.61
1:C:14:GLN:NE2	1:C:459:GLU:OE2	2.33	0.61
1:B:166:THR:O	1:B:211:GLY:N	2.23	0.61
1:B:44:PRO:HD3	1:B:155:ASP:HA	1.82	0.61
1:B:118:MET:N	1:B:118:MET:SD	2.73	0.61
1:C:221:LEU:HD13	1:C:223:ILE:HD11	1.83	0.60
1:A:334:GLU:HG2	1:A:335:GLN:HG3	1.81	0.60
1:B:42:ARG:NH1	1:B:54:TYR:OH	2.33	0.60
1:B:127:PRO:HB3	1:B:231:LEU:HD13	1.84	0.60
1:D:147:LEU:HD22	1:D:240:PHE:HZ	1.67	0.60
1:C:123:LEU:HB2	1:C:163:VAL:HG12	1.84	0.59
1:C:356:LEU:HD21	1:C:371:VAL:HG21	1.85	0.59
1:A:123:LEU:HB2	1:A:163:VAL:HG12	1.85	0.58
1:C:22:PHE:HE2	1:C:164:LEU:HD12	1.68	0.58
1:B:83:TYR:CD2	1:B:133:LEU:HD12	2.39	0.58
1:B:220:GLN:O	1:B:230:LEU:HB2	2.04	0.58
1:B:43:LYS:NZ	1:B:330:GLU:OE2	2.30	0.58
1:C:66:GLU:HB3	1:C:67:PRO:HD3	1.86	0.58
1:D:157:VAL:N	1:D:239:THR:HG21	2.12	0.58
1:C:306:ARG:O	1:C:310:GLN:HG2	2.02	0.58
1:C:47:SER:HB2	1:C:293:GLU:OE2	2.04	0.57
1:A:169:GLU:HG3	1:A:209:PRO:HA	1.85	0.57
1:A:127:PRO:HA	1:A:130:TRP:HD1	1.68	0.57
1:B:141:GLN:HG2	1:B:142:PRO:HD3	1.86	0.57
1:B:424:PRO:HG2	1:B:427:LEU:HB2	1.87	0.57
1:C:393:LEU:HD23	1:C:398:LEU:HD11	1.87	0.57
1:D:286:ASP:O	1:D:289:GLY:N	2.38	0.56
1:A:10:ARG:HH21	1:A:465:ARG:HE	1.53	0.56
1:B:150:LEU:O	1:B:154:GLY:N	2.32	0.56
1:B:63:ASP:O	1:B:140:ARG:NH2	2.36	0.56
1:C:65:LEU:HD22	1:C:137:ARG:HG3	1.87	0.56
1:C:375:LEU:O	1:C:379:THR:N	2.35	0.56
1:D:158:TYR:HB3	1:D:218:VAL:HB	1.87	0.56
1:A:222:VAL:HG12	1:A:239:THR:HA	1.86	0.56
1:A:424:PRO:HG2	1:A:427:LEU:HB2	1.88	0.55
1:D:150:LEU:O	1:D:154:GLY:N	2.34	0.55
1:D:22:PHE:CE2	1:D:164:LEU:HD12	2.41	0.55
1:B:37:TYR:HB3	1:B:61:ILE:HD12	1.89	0.55
1:D:22:PHE:HE2	1:D:164:LEU:HD12	1.70	0.55
1:B:305:ASP:HB2	1:B:308:LEU:HD23	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASP:N	1:A:126:ASP:OD1	2.39	0.54
1:B:292:ALA:O	1:B:296:THR:OG1	2.25	0.54
1:D:54:TYR:HE2	1:D:218:VAL:HG21	1.72	0.54
1:C:49:PHE:CE2	1:C:290:LEU:HB2	2.43	0.54
1:D:356:LEU:HD11	1:D:371:VAL:HG11	1.89	0.54
1:B:172:VAL:H	1:B:206:VAL:HG22	1.72	0.54
1:B:47:SER:HB2	1:B:293:GLU:OE2	2.07	0.54
1:B:382:SER:HB3	1:B:465:ARG:HH22	1.72	0.53
1:D:221:LEU:O	1:D:239:THR:HG22	2.08	0.53
1:A:10:ARG:NH2	1:A:465:ARG:HE	2.06	0.53
1:A:67:PRO:HG2	1:A:137:ARG:HB3	1.91	0.53
1:A:285:GLU:HB2	1:A:289:GLY:HA3	1.88	0.53
1:A:220:GLN:O	1:A:230:LEU:HB2	2.09	0.53
1:B:223:ILE:HB	1:B:240:PHE:CZ	2.44	0.53
1:C:61:ILE:HD12	1:C:159:VAL:HG11	1.90	0.53
1:C:382:SER:N	1:C:385:GLN:OE1	2.33	0.53
1:C:357:VAL:HG12	1:C:363:LEU:HD23	1.90	0.53
1:C:284:THR:HB	1:C:289:GLY:HA3	1.91	0.53
1:C:421:MET:HE3	1:C:458:TRP:HB2	1.91	0.53
1:C:439:TRP:CD2	1:C:449:LEU:HD12	2.44	0.53
1:A:393:LEU:HD23	1:A:398:LEU:HD13	1.92	0.52
1:C:22:PHE:CE2	1:C:164:LEU:HD12	2.45	0.52
1:B:385:GLN:HG2	1:B:441:LEU:HD12	1.92	0.52
1:C:166:THR:HG22	1:C:214:LEU:HD11	1.92	0.52
1:C:130:TRP:CZ3	1:C:229:VAL:HG11	2.45	0.52
1:D:231:LEU:O	1:D:233:PRO:HD3	2.10	0.51
1:C:127:PRO:HA	1:C:130:TRP:HD1	1.75	0.51
1:D:90:ILE:HG23	1:D:121:TYR:HE1	1.76	0.51
1:A:48:TRP:CZ3	1:A:284:THR:HA	2.46	0.51
1:B:18:HIS:HB2	1:B:460:PRO:HG2	1.91	0.51
1:B:91:GLN:HB2	1:B:120:VAL:HG23	1.93	0.51
1:D:53:ARG:HH12	1:D:55:LYS:HE2	1.76	0.51
1:A:157:VAL:HG22	1:A:239:THR:HG21	1.93	0.50
1:A:65:LEU:C	1:A:140:ARG:HB2	2.32	0.50
1:C:13:VAL:HA	1:C:16:LEU:HB3	1.93	0.50
1:A:398:LEU:H	1:A:398:LEU:HD23	1.77	0.50
1:A:69:ALA:HB3	1:A:137:ARG:HH22	1.77	0.50
1:A:365:PRO:HA	1:A:368:ALA:HB3	1.94	0.50
1:C:41:VAL:HG22	1:C:57:VAL:HG22	1.94	0.50
1:B:363:LEU:H	1:B:363:LEU:HD23	1.77	0.50
1:A:345:LEU:O	1:A:350:GLY:HA3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLN:HA	1:A:460:PRO:CB	2.41	0.49
1:A:385:GLN:HG2	1:A:441:LEU:HD12	1.94	0.49
1:A:93:SER:OG	1:A:95:GLU:OE2	2.23	0.49
1:C:320:LEU:HB2	1:C:390:ALA:HB2	1.94	0.49
1:D:241:GLN:N	1:D:241:GLN:OE1	2.46	0.49
1:C:345:LEU:O	1:C:350:GLY:HA3	2.12	0.49
1:A:472:SER:O	1:A:476:LEU:HG	2.12	0.49
1:D:123:LEU:HB2	1:D:163:VAL:HG12	1.94	0.49
1:A:49:PHE:HE2	1:A:290:LEU:HB2	1.76	0.49
1:A:9:VAL:O	1:A:13:VAL:HG22	2.13	0.48
1:B:393:LEU:HD21	1:B:476:LEU:HD13	1.94	0.48
1:C:148:GLN:HA	1:C:151:ARG:HG2	1.95	0.48
1:D:345:LEU:O	1:D:350:GLY:HA3	2.13	0.48
1:C:88:GLY:HA2	1:C:122:SER:O	2.13	0.48
1:C:356:LEU:HD11	1:C:371:VAL:HG11	1.94	0.48
1:D:22:PHE:HA	1:D:216:PHE:O	2.13	0.48
1:A:301:LEU:C	1:A:303:LEU:H	2.17	0.48
1:C:472:SER:O	1:C:476:LEU:HD13	2.12	0.48
1:A:393:LEU:HD21	1:A:476:LEU:HB3	1.96	0.48
1:A:60:SER:OG	1:A:61:ILE:N	2.47	0.48
1:C:30:SER:O	1:C:33:GLY:N	2.47	0.47
1:D:144:HIS:HA	1:D:147:LEU:HB2	1.96	0.47
1:B:235:LYS:HA	1:B:235:LYS:HD2	1.62	0.47
1:B:343:GLU:OE2	1:C:145:LYS:HG2	2.14	0.47
1:B:437:PRO:O	1:B:441:LEU:HB2	2.14	0.47
1:D:49:PHE:CE2	1:D:290:LEU:HB2	2.47	0.47
1:B:50:TRP:CH2	1:B:377:ALA:HB2	2.50	0.47
1:B:157:VAL:CG2	1:B:239:THR:HG21	2.44	0.47
1:D:42:ARG:O	1:D:42:ARG:HG3	2.13	0.47
1:D:92:GLY:HA2	1:D:119:ASN:HA	1.97	0.47
1:D:421:MET:HB2	1:D:456:VAL:CG1	2.45	0.47
1:A:441:LEU:HD21	1:A:469:LEU:HD11	1.96	0.46
1:B:404:LEU:O	1:B:408:LEU:HG	2.14	0.46
1:B:83:TYR:CE2	1:B:133:LEU:HD12	2.50	0.46
1:D:420:THR:HA	1:D:457:CYS:HA	1.97	0.46
1:B:60:SER:OG	1:B:61:ILE:N	2.48	0.46
1:C:158:TYR:CE2	1:C:220:GLN:HB2	2.50	0.46
1:C:432:TRP:HZ2	1:C:449:LEU:HD13	1.79	0.46
1:B:143:GLU:O	1:B:147:LEU:HB2	2.16	0.46
1:C:232:PHE:HB3	1:D:419:SER:HA	1.96	0.46
1:D:42:ARG:HE	1:D:54:TYR:HE1	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:HA	1:B:232:PHE:HB2	1.96	0.46
1:D:57:VAL:HG23	1:D:59:LEU:HG	1.96	0.46
1:C:42:ARG:HG3	1:C:54:TYR:CE1	2.51	0.46
1:D:441:LEU:HD21	1:D:469:LEU:HD11	1.98	0.45
1:B:60:SER:HB3	1:B:62:LYS:NZ	2.31	0.45
1:C:39:LEU:HD12	1:C:39:LEU:H	1.82	0.45
1:D:133:LEU:HG	1:D:137:ARG:HD2	1.98	0.45
1:A:332:ALA:HB1	1:A:342:VAL:HG11	1.99	0.45
1:D:425:PRO:HG3	1:D:432:TRP:CG	2.51	0.45
1:C:220:GLN:O	1:C:230:LEU:N	2.48	0.45
1:C:241:GLN:N	1:C:241:GLN:OE1	2.47	0.45
1:A:374:LEU:HD13	1:A:475:LEU:HD12	1.99	0.45
1:A:408:LEU:HD13	1:A:421:MET:HE2	1.99	0.45
1:D:312:LEU:HD11	1:D:352:VAL:HG13	1.98	0.45
1:A:84:ASP:OD1	1:A:85:ALA:N	2.49	0.44
1:B:126:ASP:OD1	1:B:129:THR:OG1	2.32	0.44
1:C:157:VAL:CG1	1:C:239:THR:HG21	2.47	0.44
1:C:441:LEU:HD21	1:C:469:LEU:HD11	1.99	0.44
1:D:374:LEU:HD13	1:D:475:LEU:HD12	1.99	0.44
1:D:313:LEU:HD23	1:D:316:LEU:HD12	2.00	0.44
1:B:67:PRO:HG3	1:B:137:ARG:HE	1.83	0.44
1:D:228:ASP:N	1:D:228:ASP:OD1	2.50	0.44
1:D:393:LEU:HD23	1:D:398:LEU:HD11	1.99	0.44
1:C:232:PHE:HB3	1:D:420:THR:H	1.83	0.44
1:D:419:SER:O	1:D:458:TRP:HB3	2.18	0.44
1:D:385:GLN:HG2	1:D:441:LEU:HD12	2.00	0.44
1:D:421:MET:SD	1:D:458:TRP:HB2	2.57	0.44
1:B:172:VAL:N	1:B:206:VAL:HG22	2.33	0.44
1:B:50:TRP:CZ2	1:B:468:ALA:HA	2.52	0.44
1:A:158:TYR:CD2	1:A:220:GLN:HB2	2.53	0.44
1:B:356:LEU:HD11	1:B:371:VAL:HG21	2.00	0.43
1:C:287:PHE:CD1	1:C:287:PHE:C	2.92	0.43
1:C:465:ARG:HG3	1:C:465:ARG:HH11	1.82	0.43
1:D:155:ASP:N	1:D:155:ASP:OD1	2.51	0.43
1:D:147:LEU:HD22	1:D:240:PHE:CZ	2.52	0.43
1:B:147:LEU:HD11	1:B:223:ILE:HG21	2.00	0.43
1:C:159:VAL:HG22	1:C:219:ALA:O	2.19	0.43
1:A:7:ARG:O	1:A:10:ARG:HB2	2.18	0.43
1:C:416:GLN:HA	1:C:460:PRO:HB3	2.00	0.43
1:C:120:VAL:HB	1:C:164:LEU:HD21	2.00	0.43
1:A:236:LYS:HE2	1:A:236:LYS:HB3	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ASN:O	1:C:132:THR:HG23	2.18	0.43
1:C:425:PRO:HG3	1:C:432:TRP:CD2	2.54	0.43
1:B:22:PHE:HA	1:B:216:PHE:O	2.19	0.43
1:C:157:VAL:HG13	1:C:239:THR:HG21	2.01	0.43
1:A:221:LEU:O	1:A:239:THR:HG23	2.19	0.42
1:D:206:VAL:HG22	1:D:207:THR:H	1.83	0.42
1:D:221:LEU:HD22	1:D:227:LEU:HD11	2.01	0.42
1:D:428:LEU:HG	1:D:429:GLY:H	1.85	0.42
1:C:49:PHE:HE2	1:C:290:LEU:HB2	1.85	0.42
1:C:451:GLU:OE1	1:C:451:GLU:N	2.53	0.42
1:B:157:VAL:HG23	1:B:239:THR:HG21	2.01	0.42
1:A:139:LEU:HG	1:A:141:GLN:HG2	2.01	0.42
1:D:158:TYR:CE2	1:D:220:GLN:HB2	2.54	0.42
1:D:55:LYS:HA	1:D:55:LYS:HD3	1.89	0.42
1:B:312:LEU:O	1:B:316:LEU:HG	2.19	0.42
1:B:382:SER:HB3	1:B:465:ARG:NH2	2.34	0.42
1:A:316:LEU:O	1:A:320:LEU:HG	2.19	0.42
1:A:34:PHE:HE1	1:A:56:CYS:HB2	1.84	0.42
1:B:452:ASP:OD2	1:B:455:HIS:ND1	2.48	0.42
1:D:424:PRO:HG2	1:D:427:LEU:HD23	2.02	0.42
1:A:66:GLU:HB2	1:A:67:PRO:HD3	2.02	0.42
1:B:92:GLY:O	1:B:119:ASN:HA	2.19	0.42
1:B:8:VAL:O	1:B:12:VAL:HG23	2.20	0.42
1:B:222:VAL:HG12	1:B:239:THR:HA	2.02	0.41
1:B:425:PRO:HG3	1:B:432:TRP:CD2	2.55	0.41
1:A:127:PRO:HA	1:A:130:TRP:CD1	2.51	0.41
1:B:67:PRO:HG3	1:B:137:ARG:NE	2.35	0.41
1:B:407:SER:CB	1:B:423:LEU:HD22	2.50	0.41
1:C:329:LEU:HB2	1:C:349:ALA:HB1	2.02	0.41
1:A:158:TYR:HA	1:A:220:GLN:HA	2.02	0.41
1:A:352:VAL:O	1:A:356:LEU:HG	2.20	0.41
1:B:146:VAL:O	1:B:150:LEU:HD22	2.20	0.41
1:B:42:ARG:HG2	1:B:52:PRO:HG2	2.02	0.41
1:B:472:SER:O	1:B:476:LEU:HG	2.21	0.41
1:B:54:TYR:CE2	1:B:218:VAL:HG11	2.55	0.41
1:B:90:ILE:HD13	1:B:121:TYR:CD1	2.55	0.41
1:B:83:TYR:HB3	1:B:84:ASP:H	1.57	0.41
1:B:381:LEU:HD11	1:B:469:LEU:HA	2.02	0.41
1:D:236:LYS:NZ	1:D:236:LYS:HB3	2.35	0.41
1:C:94:VAL:HG22	1:D:89:GLN:H	1.84	0.41
1:D:40:VAL:HG23	1:D:158:TYR:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HB2	1:A:163:VAL:CG1	2.50	0.41
1:A:330:GLU:O	1:A:334:GLU:HB2	2.21	0.41
1:A:333:LEU:HD11	1:A:363:LEU:HD22	2.02	0.41
1:C:439:TRP:CE2	1:C:449:LEU:HD12	2.56	0.41
1:D:43:LYS:H	1:D:43:LYS:HG2	1.59	0.41
1:D:472:SER:O	1:D:476:LEU:HG	2.20	0.41
1:C:389:LEU:HD23	1:C:389:LEU:HA	1.83	0.41
1:D:39:LEU:H	1:D:39:LEU:HD12	1.86	0.41
1:A:420:THR:H	1:B:232:PHE:HB3	1.86	0.41
1:A:39:LEU:H	1:A:39:LEU:HD12	1.86	0.41
1:B:13:VAL:HG12	1:B:461:GLN:HE21	1.86	0.41
1:B:17:ASP:N	1:B:17:ASP:OD1	2.54	0.41
1:D:298:SER:O	1:D:302:GLU:N	2.53	0.41
1:A:231:LEU:O	1:A:233:PRO:HD3	2.21	0.41
1:B:129:THR:HA	1:B:132:THR:HG22	2.02	0.41
1:B:42:ARG:CG	1:B:52:PRO:HG2	2.51	0.41
1:C:31:SER:HB2	1:C:213:THR:O	2.21	0.41
1:A:222:VAL:HA	1:A:239:THR:HG23	2.03	0.40
1:C:473:LEU:HD23	1:C:473:LEU:HA	1.94	0.40
1:D:362:MET:SD	1:D:362:MET:N	2.94	0.40
1:A:228:ASP:N	1:A:228:ASP:OD1	2.54	0.40
1:B:121:TYR:CG	1:B:122:SER:N	2.89	0.40
1:C:146:VAL:O	1:C:150:LEU:HG	2.22	0.40
1:C:63:ASP:N	1:C:63:ASP:OD1	2.54	0.40
1:A:235:LYS:HA	1:A:235:LYS:HD2	1.81	0.40
1:B:395:SER:OG	1:B:397:THR:HG22	2.22	0.40
1:A:148:GLN:HA	1:A:151:ARG:HG2	2.02	0.40
1:B:365:PRO:O	1:B:369:ILE:HG12	2.22	0.40
1:C:169:GLU:HA	1:C:208:ILE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	361/485 (74%)	327 (91%)	34 (9%)	0	100	100
1	B	359/485 (74%)	322 (90%)	37 (10%)	0	100	100
1	C	369/485 (76%)	341 (92%)	28 (8%)	0	100	100
1	D	367/485 (76%)	332 (90%)	35 (10%)	0	100	100
All	All	1456/1940 (75%)	1322 (91%)	134 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	323/410 (79%)	307 (95%)	16 (5%)	24	58
1	B	322/410 (78%)	295 (92%)	27 (8%)	11	40
1	C	327/410 (80%)	309 (94%)	18 (6%)	21	54
1	D	327/410 (80%)	305 (93%)	22 (7%)	16	48
All	All	1299/1640 (79%)	1216 (94%)	83 (6%)	17	50

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	32	THR
1	A	94	VAL
1	A	118	MET
1	A	126	ASP
1	A	144	HIS
1	A	145	LYS
1	A	171	GLU
1	A	304	LEU
1	A	335	GLN
1	A	337	GLN
1	A	339	LEU
1	A	343	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	375	LEU
1	A	408	LEU
1	A	465	ARG
1	B	17	ASP
1	B	27	SER
1	B	48	TRP
1	B	49	PHE
1	B	56	CYS
1	B	62	LYS
1	B	63	ASP
1	B	64	ILE
1	B	118	MET
1	B	129	THR
1	B	144	HIS
1	B	150	LEU
1	B	157	VAL
1	B	205	THR
1	B	239	THR
1	B	284	THR
1	B	288	GLN
1	B	296	THR
1	B	337	GLN
1	B	362	MET
1	B	363	LEU
1	B	398	LEU
1	B	416	GLN
1	B	452	ASP
1	B	453	THR
1	B	455	HIS
1	B	456	VAL
1	C	41	VAL
1	C	42	ARG
1	C	43	LYS
1	C	48	TRP
1	C	57	VAL
1	C	132	THR
1	C	140	ARG
1	C	143	GLU
1	C	149	GLN
1	C	157	VAL
1	C	231	LEU
1	C	240	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	288	GLN
1	C	329	LEU
1	C	334	GLU
1	C	337	GLN
1	C	452	ASP
1	C	476	LEU
1	D	11	ARG
1	D	21	GLU
1	D	42	ARG
1	D	43	LYS
1	D	48	TRP
1	D	84	ASP
1	D	91	GLN
1	D	126	ASP
1	D	155	ASP
1	D	173	THR
1	D	205	THR
1	D	224	ASP
1	D	230	LEU
1	D	231	LEU
1	D	284	THR
1	D	285	GLU
1	D	334	GLU
1	D	337	GLN
1	D	362	MET
1	D	375	LEU
1	D	421	MET
1	D	456	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	ASN
1	A	463	GLN
1	B	463	GLN
1	D	323	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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	371/485 (76%)	0.24	21 (5%) 23 21	133, 205, 267, 301	0
1	B	369/485 (76%)	0.19	19 (5%) 28 25	104, 176, 254, 289	0
1	C	379/485 (78%)	-0.00	6 (1%) 72 66	103, 160, 224, 271	0
1	D	377/485 (77%)	0.14	17 (4%) 33 29	95, 174, 245, 282	0
All	All	1496/1940 (77%)	0.14	63 (4%) 36 32	95, 179, 254, 301	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	336	GLY	5.3
1	D	335	GLN	5.2
1	A	305	ASP	4.9
1	B	424	PRO	4.8
1	A	363	LEU	4.8
1	D	337	GLN	4.6
1	A	425	PRO	4.4
1	A	453	THR	4.2
1	D	341	PRO	4.0
1	D	479	LEU	3.9
1	C	425	PRO	3.9
1	B	228	ASP	3.9
1	A	37	TYR	3.8
1	D	338	SER	3.5
1	A	430	ASN	3.5
1	A	167	GLN	3.4
1	B	425	PRO	3.2
1	B	428	LEU	3.2
1	A	226	ASP	3.1
1	A	432	TRP	3.1
1	C	148	GLN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	207	THR	2.9
1	A	428	LEU	2.8
1	B	430	ASN	2.7
1	C	37	TYR	2.7
1	D	340	GLY	2.6
1	B	57	VAL	2.6
1	D	342	VAL	2.6
1	A	67	PRO	2.6
1	A	171	GLU	2.6
1	B	335	GLN	2.6
1	C	144	HIS	2.6
1	B	229	VAL	2.5
1	B	427	LEU	2.5
1	A	121	TYR	2.4
1	D	228	ASP	2.4
1	B	423	LEU	2.4
1	A	429	GLY	2.3
1	C	172	VAL	2.3
1	D	363	LEU	2.3
1	B	58	ASN	2.3
1	D	432	TRP	2.3
1	B	59	LEU	2.3
1	D	226	ASP	2.3
1	B	146	VAL	2.3
1	A	366	GLU	2.2
1	B	212	SER	2.2
1	B	359	SER	2.2
1	D	429	GLY	2.2
1	A	364	VAL	2.2
1	D	283	PHE	2.2
1	B	161	THR	2.2
1	A	66	GLU	2.2
1	D	480	SER	2.1
1	A	212	SER	2.1
1	B	421	MET	2.1
1	C	455	HIS	2.1
1	B	133	LEU	2.1
1	A	339	LEU	2.0
1	A	154	GLY	2.0
1	B	37	TYR	2.0
1	D	474	ALA	2.0
1	D	303	LEU	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 carbohydrates 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.