



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2024 – 05:11 AM EST

PDB ID : 4LGI
Title : N-terminal truncated NleC structure
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Deposited on : 2013-06-28
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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)	:	2.39

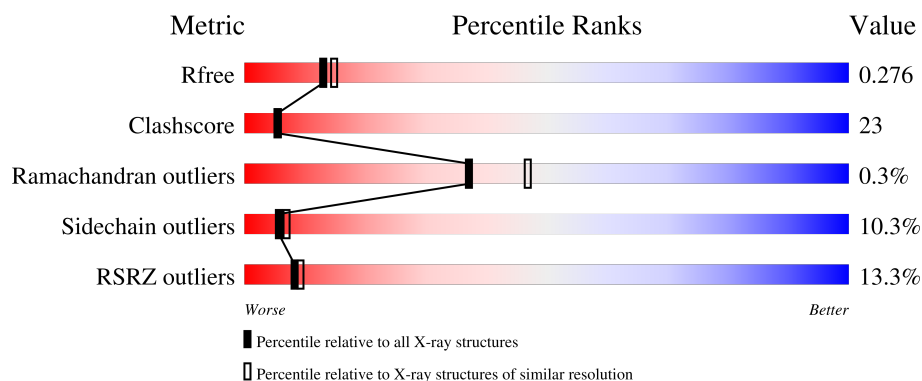
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	264	<div> <div>9%</div> <div>48%</div> <div>28%</div> <div>5%</div> <div>20%</div> </div>
1	B	264	<div> <div>8%</div> <div>53%</div> <div>22%</div> <div>•</div> <div>22%</div> </div>
1	C	264	<div> <div>11%</div> <div>50%</div> <div>25%</div> <div>•</div> <div>21%</div> </div>
1	D	264	<div> <div>14%</div> <div>45%</div> <div>28%</div> <div>6%</div> <div>22%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6801 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	Se	0	0	0
			1664	1029	293	336	3	3			
1	B	206	Total	C	N	O	S	Se	0	0	0
			1641	1017	291	327	3	3			
1	C	208	Total	C	N	O	S	Se	0	0	0
			1633	1011	289	327	3	3			
1	D	206	Total	C	N	O	S	Se	0	0	0
			1610	998	287	319	3	3			

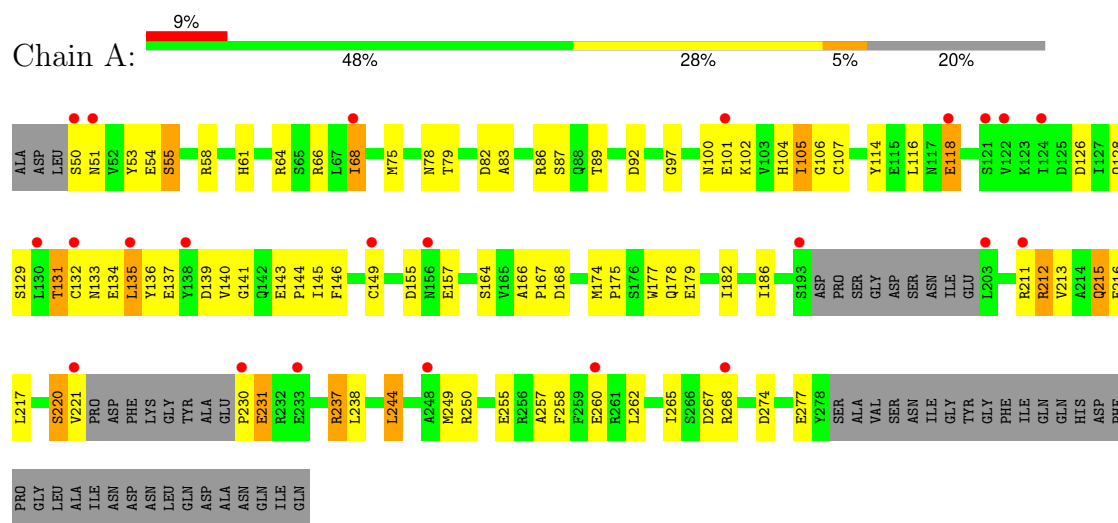
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	0
			68	68		
2	B	61	Total	O	0	0
			61	61		
2	C	73	Total	O	0	0
			73	73		
2	D	51	Total	O	0	0
			51	51		

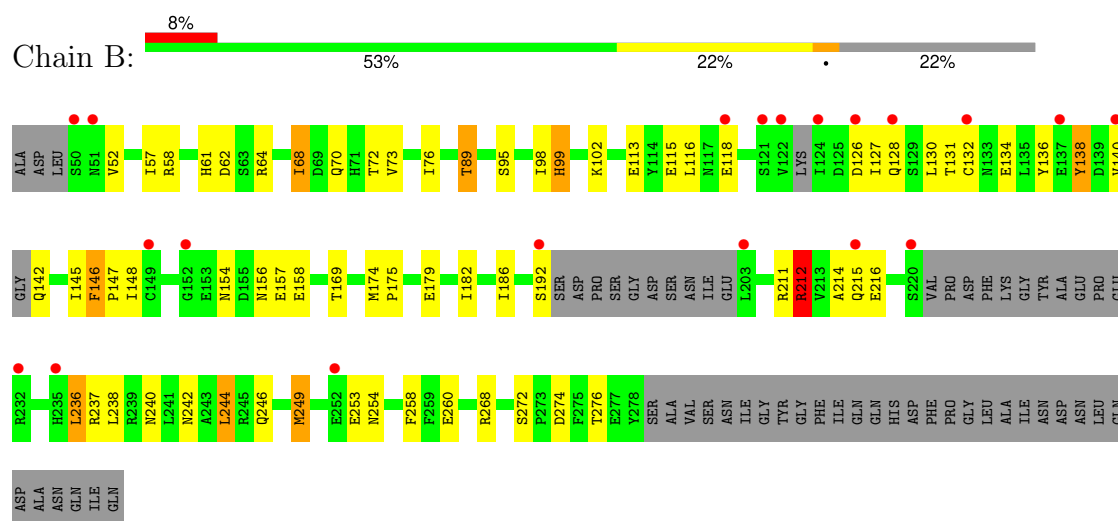
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Uncharacterized protein

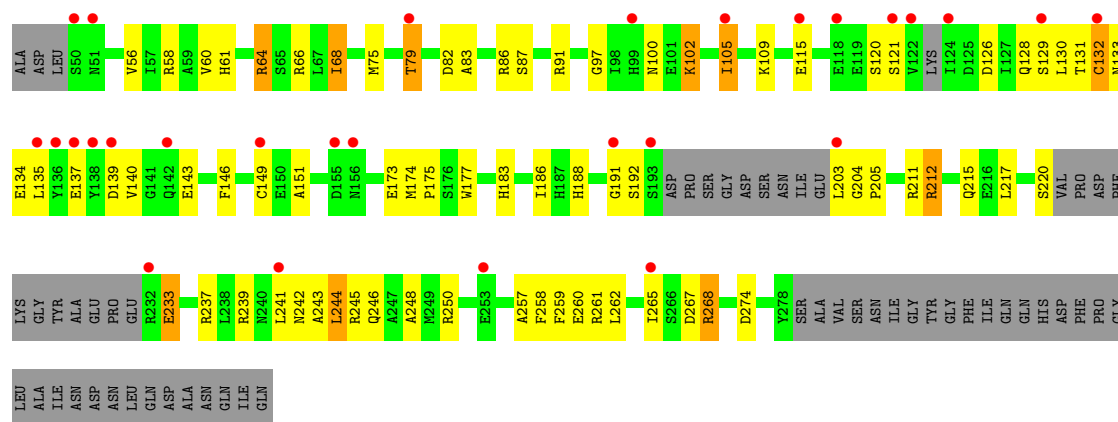


• Molecule 1: Uncharacterized protein

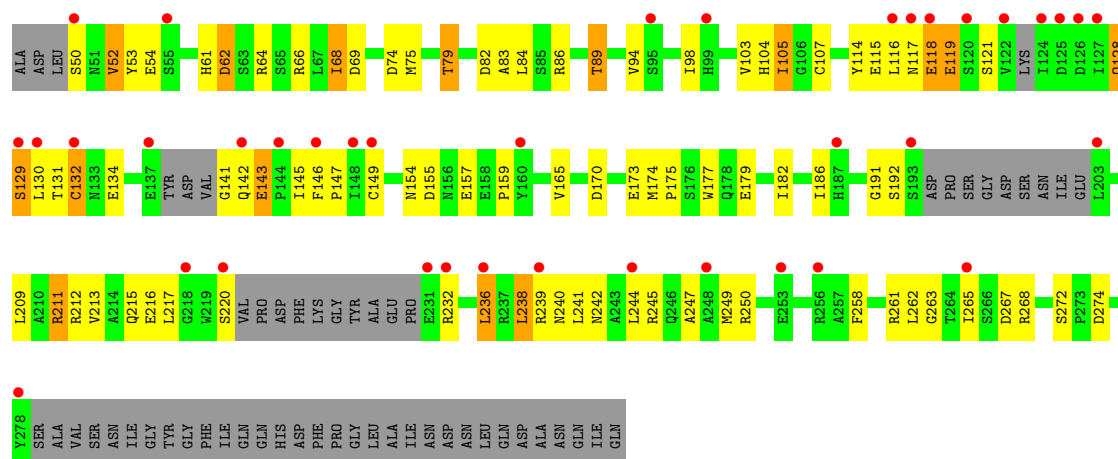
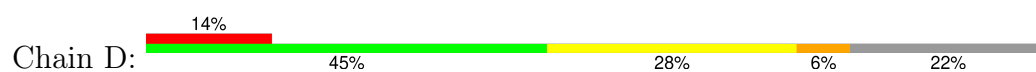


• Molecule 1: Uncharacterized protein





● Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.51Å 88.66Å 110.65Å 90.00° 92.89° 90.00°	Depositor
Resolution (Å)	37.61 – 2.30 37.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (37.61-2.30) 99.4 (37.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.253 , 0.280 0.248 , 0.276	Depositor DCC
R_{free} test set	2571 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6801	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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	0.67	0/1693	0.67	2/2293 (0.1%)
1	B	0.72	0/1669	0.67	2/2256 (0.1%)
1	C	0.66	0/1661	0.61	0/2248
1	D	0.63	0/1637	0.60	0/2214
All	All	0.67	0/6660	0.64	4/9011 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ILE	CB-CA-C	-5.95	99.70	111.60
1	A	230	PRO	N-CA-CB	5.60	110.02	103.30
1	B	212	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	126	ASP	CB-CG-OD1	5.01	122.81	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	1664	0	1516	83	1
1	B	1641	0	1507	55	0
1	C	1633	0	1489	62	0
1	D	1610	0	1467	94	0
2	A	68	0	0	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	61	0	0	16	0
2	C	73	0	0	19	0
2	D	51	0	0	32	1
All	All	6801	0	5979	292	1

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 23.

All (292) 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:131:THR:CG2	1:C:134:GLU:OE1	1.69	1.39
1:D:98:ILE:HG22	2:D:435:HOH:O	1.31	1.23
1:A:166:ALA:HA	2:A:424:HOH:O	1.39	1.17
1:C:244:LEU:N	2:C:448:HOH:O	1.80	1.14
1:C:203:LEU:N	2:C:463:HOH:O	1.83	1.11
1:C:149:CYS:SG	2:C:406:HOH:O	2.11	1.09
1:D:98:ILE:C	2:D:435:HOH:O	1.91	1.09
1:A:167:PRO:CD	2:A:424:HOH:O	2.02	1.08
1:B:131:THR:HG22	1:B:134:GLU:OE1	1.54	1.08
1:A:157:GLU:HB3	2:A:468:HOH:O	1.53	1.07
1:D:52:VAL:N	2:D:413:HOH:O	1.82	1.07
1:C:212:ARG:HH11	1:C:212:ARG:HG3	1.19	1.05
1:A:177:TRP:CD1	2:A:424:HOH:O	2.10	1.05
1:B:89:THR:HG22	1:B:216:GLU:OE2	1.57	1.04
1:C:212:ARG:HG3	1:C:212:ARG:NH1	1.71	1.03
1:D:116:LEU:N	2:D:432:HOH:O	1.80	1.00
1:C:242:ASN:C	2:C:448:HOH:O	2.00	0.99
1:A:118:GLU:N	1:A:118:GLU:OE1	1.93	0.98
1:A:141:GLY:HA2	1:A:237:ARG:NH2	1.78	0.97
1:A:131:THR:HG23	1:A:134:GLU:CD	1.83	0.97
1:C:131:THR:HG22	1:C:134:GLU:OE1	0.80	0.97
1:A:167:PRO:HD3	2:A:424:HOH:O	1.60	0.96
1:A:177:TRP:CE2	2:A:424:HOH:O	2.18	0.95
1:C:140:VAL:HA	1:C:143:GLU:OE2	1.65	0.95
1:D:238:LEU:O	1:D:242:ASN:ND2	2.00	0.94
1:C:220:SER:C	2:C:436:HOH:O	2.05	0.94
1:B:254:ASN:ND2	2:B:452:HOH:O	1.99	0.93
1:B:268:ARG:NH2	2:B:441:HOH:O	1.92	0.93
1:D:50:SER:N	2:D:413:HOH:O	2.00	0.93
1:D:115:GLU:CA	2:D:432:HOH:O	2.16	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ARG:O	2:C:449:HOH:O	1.86	0.91
1:A:89:THR:OG1	1:A:216:GLU:OE2	1.89	0.91
1:D:115:GLU:HA	2:D:432:HOH:O	1.71	0.91
1:B:253:GLU:CB	2:B:452:HOH:O	2.18	0.90
1:A:131:THR:HG23	1:A:134:GLU:OE1	1.71	0.90
1:D:75:MSE:O	1:D:79:THR:HG23	1.71	0.89
1:B:260:GLU:OE2	2:B:439:HOH:O	1.88	0.89
1:B:272:SER:OG	2:B:435:HOH:O	1.88	0.89
1:A:177:TRP:NE1	2:A:424:HOH:O	2.00	0.88
1:D:52:VAL:HG22	2:D:413:HOH:O	1.73	0.88
1:B:89:THR:CG2	1:B:216:GLU:OE2	2.21	0.88
1:C:241:LEU:O	2:C:448:HOH:O	1.90	0.88
1:D:131:THR:HG22	1:D:134:GLU:OE1	1.73	0.87
1:D:98:ILE:O	2:D:435:HOH:O	1.88	0.87
1:A:155:ASP:OD2	2:A:461:HOH:O	1.91	0.87
1:C:133:ASN:HB2	2:C:468:HOH:O	1.76	0.86
1:A:126:ASP:OD1	1:A:129:SER:OG	1.93	0.85
1:D:132:CYS:SG	2:D:410:HOH:O	2.35	0.85
1:A:149:CYS:SG	2:A:416:HOH:O	2.35	0.85
1:C:133:ASN:CB	2:C:468:HOH:O	2.25	0.84
1:C:109:LYS:NZ	2:C:466:HOH:O	2.10	0.84
1:D:50:SER:HA	1:D:53:TYR:HD2	1.42	0.84
1:A:211:ARG:O	1:A:215:GLN:HG2	1.78	0.84
1:B:240:ASN:O	2:B:407:HOH:O	1.95	0.83
1:C:220:SER:O	2:C:436:HOH:O	1.97	0.83
1:D:220:SER:O	2:D:421:HOH:O	1.96	0.83
1:D:131:THR:CG2	1:D:134:GLU:HG3	2.10	0.81
1:D:66:ARG:CG	2:D:431:HOH:O	2.29	0.81
1:C:212:ARG:HH11	1:C:212:ARG:CG	1.94	0.81
1:D:52:VAL:CA	2:D:413:HOH:O	2.21	0.81
1:C:115:GLU:OE1	2:C:433:HOH:O	1.98	0.80
1:D:118:GLU:OE1	2:D:424:HOH:O	1.99	0.80
1:A:87:SER:OG	2:A:454:HOH:O	1.99	0.78
1:A:131:THR:CG2	1:A:134:GLU:CD	2.52	0.77
1:D:66:ARG:HG2	2:D:431:HOH:O	1.86	0.76
1:D:241:LEU:HD21	1:D:245:ARG:NH1	2.00	0.76
1:A:177:TRP:CG	2:A:424:HOH:O	2.34	0.76
1:D:141:GLY:N	2:D:447:HOH:O	2.18	0.76
1:A:79:THR:HG22	1:A:178:GLN:HE21	1.49	0.76
1:D:62:ASP:OD1	2:D:417:HOH:O	2.02	0.75
1:A:167:PRO:HD2	2:A:424:HOH:O	1.73	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:OE1	2:B:447:HOH:O	2.03	0.75
1:B:62:ASP:OD1	2:B:423:HOH:O	2.05	0.75
1:B:89:THR:HG22	1:B:216:GLU:CD	2.06	0.75
1:A:177:TRP:CD2	2:A:424:HOH:O	2.37	0.75
1:D:131:THR:HG23	1:D:134:GLU:HG3	1.69	0.75
1:D:89:THR:HG23	1:D:216:GLU:OE2	1.87	0.74
1:B:276:THR:HG23	2:B:435:HOH:O	1.87	0.74
1:D:52:VAL:CB	2:D:413:HOH:O	2.36	0.73
1:A:141:GLY:HA2	1:A:237:ARG:HH21	1.54	0.72
1:B:89:THR:CG2	1:B:216:GLU:CD	2.59	0.70
1:D:66:ARG:N	2:D:431:HOH:O	2.24	0.70
1:A:75:MSE:O	1:A:79:THR:HG23	1.91	0.70
1:B:89:THR:CG2	1:B:216:GLU:OE1	2.40	0.70
1:A:89:THR:N	2:A:454:HOH:O	2.10	0.69
1:D:52:VAL:CG2	2:D:413:HOH:O	2.37	0.68
1:A:131:THR:CG2	1:A:134:GLU:OE1	2.42	0.68
1:A:216:GLU:OE1	2:A:454:HOH:O	2.13	0.67
1:D:114:TYR:CD2	1:D:145:ILE:HD12	2.30	0.67
1:C:267:ASP:O	1:C:268:ARG:HB2	1.94	0.67
1:A:157:GLU:OE1	2:A:468:HOH:O	2.12	0.66
1:B:274:ASP:HB2	2:B:435:HOH:O	1.94	0.66
1:A:141:GLY:CA	1:A:237:ARG:HH21	2.07	0.66
1:B:174:MSE:HB3	1:B:175:PRO:HD3	1.78	0.66
1:C:75:MSE:O	1:C:79:THR:HG23	1.94	0.66
1:A:89:THR:CB	2:A:454:HOH:O	2.44	0.66
1:A:141:GLY:O	2:A:436:HOH:O	2.14	0.64
1:D:261:ARG:NH1	1:D:272:SER:O	2.25	0.64
1:D:241:LEU:HD21	1:D:245:ARG:CZ	2.28	0.63
1:C:68:ILE:HD13	1:C:258:PHE:CE1	2.33	0.63
1:B:89:THR:HG23	1:B:216:GLU:OE1	1.99	0.62
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.65	0.61
1:B:57:ILE:O	2:B:429:HOH:O	2.16	0.61
1:C:183:HIS:HA	1:C:186:ILE:HD12	1.83	0.60
1:D:170:ASP:OD2	2:D:407:HOH:O	2.16	0.60
1:A:135:LEU:HD21	1:A:244:LEU:HD13	1.84	0.60
1:C:102:LYS:HE2	1:C:191:GLY:HA3	1.82	0.60
1:A:174:MSE:HB3	1:A:175:PRO:HD3	1.83	0.59
1:B:156:ASN:O	1:B:157:GLU:HB2	2.02	0.59
1:B:157:GLU:HB3	2:B:446:HOH:O	2.01	0.59
1:A:68:ILE:CD1	1:A:258:PHE:CE2	2.86	0.59
1:A:68:ILE:HD11	1:A:258:PHE:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HD11	1:A:244:LEU:HD11	1.84	0.59
1:D:238:LEU:HD23	2:D:428:HOH:O	2.01	0.58
1:C:133:ASN:N	2:C:468:HOH:O	2.05	0.58
1:D:142:GLN:N	2:D:447:HOH:O	2.35	0.58
1:D:52:VAL:HG13	2:D:413:HOH:O	2.02	0.58
1:D:68:ILE:HD11	1:D:258:PHE:CE1	2.38	0.58
1:A:54:GLU:OE1	1:A:58:ARG:NH1	2.37	0.57
1:D:130:LEU:HD23	1:D:134:GLU:CD	2.25	0.57
1:A:50:SER:N	2:A:452:HOH:O	2.36	0.57
1:C:211:ARG:O	1:C:215:GLN:HG3	2.03	0.57
1:D:66:ARG:HG3	2:D:431:HOH:O	2.00	0.57
1:A:212:ARG:HG3	1:A:212:ARG:NH1	2.20	0.57
1:B:138:TYR:CD1	1:B:138:TYR:N	2.73	0.57
1:B:212:ARG:HG3	1:B:212:ARG:HH11	1.70	0.57
1:D:129:SER:O	1:D:129:SER:OG	2.18	0.57
1:C:100:ASN:ND2	2:C:423:HOH:O	2.12	0.56
1:A:133:ASN:O	1:A:137:GLU:CB	2.52	0.56
1:C:126:ASP:OD2	1:C:129:SER:N	2.38	0.56
1:B:89:THR:HG22	1:B:216:GLU:OE1	2.05	0.56
1:B:145:ILE:HD11	1:B:244:LEU:HD11	1.88	0.56
1:D:69:ASP:OD2	1:D:250:ARG:NH1	2.21	0.56
1:B:61:HIS:O	1:B:64:ARG:HD3	2.04	0.56
1:D:155:ASP:HB2	2:D:419:HOH:O	2.06	0.56
1:C:126:ASP:OD2	1:C:128:GLN:HB2	2.06	0.56
1:A:97:GLY:HA2	1:A:102:LYS:HB2	1.86	0.55
1:B:254:ASN:CG	2:B:452:HOH:O	2.40	0.55
1:D:103:VAL:HG13	1:D:159:PRO:HG3	1.89	0.55
1:D:141:GLY:HA2	1:D:143:GLU:OE2	2.06	0.55
1:B:142:GLN:HB2	1:B:237:ARG:HH21	1.70	0.55
1:A:220:SER:C	2:A:467:HOH:O	2.45	0.55
1:C:82:ASP:OD1	1:C:86:ARG:HD3	2.05	0.55
1:C:245:ARG:N	2:C:448:HOH:O	1.99	0.55
1:A:141:GLY:CA	1:A:237:ARG:NH2	2.58	0.55
1:A:55:SER:HB3	1:A:106:GLY:HA3	1.88	0.54
1:B:212:ARG:HG3	1:B:212:ARG:NH1	2.21	0.54
1:A:132:CYS:SG	1:A:255:GLU:HG3	2.48	0.54
1:D:117:ASN:OD1	1:D:119:GLU:HG2	2.08	0.54
1:A:212:ARG:O	1:A:216:GLU:HG3	2.07	0.54
1:B:154:ASN:C	1:B:154:ASN:OD1	2.44	0.54
1:D:261:ARG:O	1:D:265:ILE:HG13	2.07	0.54
1:A:66:ARG:HA	1:A:265:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:HG13	1:D:105:ILE:HG12	1.89	0.54
1:A:141:GLY:N	1:A:237:ARG:HH21	2.06	0.53
1:D:155:ASP:CB	2:D:419:HOH:O	2.55	0.53
1:D:128:GLN:NE2	1:D:267:ASP:OD2	2.42	0.53
1:B:242:ASN:O	1:B:246:GLN:HG3	2.10	0.52
1:B:127:ILE:O	1:B:130:LEU:HB2	2.10	0.52
1:A:64:ARG:NH2	1:A:274:ASP:OD1	2.43	0.52
1:D:128:GLN:HG2	1:D:263:GLY:HA3	1.92	0.52
1:A:220:SER:O	1:A:221:VAL:CB	2.58	0.51
1:C:267:ASP:O	1:C:268:ARG:CB	2.57	0.51
1:C:75:MSE:O	1:C:79:THR:CG2	2.58	0.51
1:B:113:GLU:HB3	1:B:148:ILE:HD12	1.92	0.51
1:D:82:ASP:OD1	1:D:86:ARG:HD3	2.11	0.51
1:A:89:THR:HB	2:A:454:HOH:O	2.07	0.51
1:A:131:THR:HG23	1:A:134:GLU:CG	2.41	0.51
1:B:154:ASN:ND2	1:B:158:GLU:OE1	2.30	0.51
1:D:238:LEU:HG	1:D:242:ASN:HD21	1.76	0.51
1:A:133:ASN:O	1:A:137:GLU:N	2.44	0.50
1:B:70:GLN:O	1:B:73:VAL:HB	2.11	0.50
1:D:52:VAL:CG1	2:D:413:HOH:O	2.58	0.50
1:D:114:TYR:CZ	1:D:147:PRO:HB3	2.46	0.50
1:A:104:HIS:HB3	1:A:107:CYS:SG	2.51	0.50
1:D:68:ILE:HD11	1:D:258:PHE:CD1	2.46	0.50
1:A:211:ARG:NH1	2:A:467:HOH:O	2.00	0.50
1:D:75:MSE:O	1:D:79:THR:CG2	2.51	0.50
1:D:64:ARG:NH2	1:D:274:ASP:OD1	2.44	0.50
1:D:61:HIS:O	1:D:64:ARG:HD3	2.12	0.49
1:D:104:HIS:HB3	1:D:107:CYS:SG	2.52	0.49
1:C:61:HIS:O	1:C:64:ARG:HD3	2.13	0.49
1:D:182:ILE:HG22	1:D:186:ILE:HD12	1.93	0.49
1:A:179:GLU:OE2	1:A:211:ARG:HD2	2.13	0.48
1:A:267:ASP:O	1:A:268:ARG:HB2	2.13	0.48
1:B:136:TYR:N	1:B:136:TYR:CD1	2.81	0.48
1:D:174:MSE:HB3	1:D:175:PRO:HD3	1.94	0.48
1:D:50:SER:HA	1:D:53:TYR:CD2	2.34	0.48
1:A:68:ILE:HD12	1:A:258:PHE:CE2	2.49	0.48
1:A:104:HIS:O	1:A:107:CYS:HB2	2.13	0.48
1:D:66:ARG:C	1:D:265:ILE:HD13	2.34	0.48
1:A:141:GLY:H	1:A:237:ARG:HH21	1.62	0.48
1:D:212:ARG:NH2	2:D:430:HOH:O	1.84	0.48
1:A:140:VAL:HG13	1:A:237:ARG:HE	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:HG22	1:A:186:ILE:HD11	1.96	0.47
1:D:145:ILE:HD11	1:D:244:LEU:HD11	1.96	0.47
1:C:174:MSE:HB3	1:C:175:PRO:HD3	1.95	0.47
1:D:75:MSE:HG3	1:D:174:MSE:HE1	1.95	0.47
1:D:191:GLY:HA2	2:D:412:HOH:O	2.15	0.47
1:D:241:LEU:CD2	1:D:245:ARG:NH1	2.77	0.47
1:A:136:TYR:N	1:A:136:TYR:CD1	2.81	0.47
1:B:182:ILE:O	1:B:186:ILE:HG13	2.15	0.47
1:C:120:SER:OG	1:C:121:SER:N	2.48	0.47
1:D:239:ARG:NH2	1:D:240:ASN:OD1	2.29	0.47
1:B:64:ARG:NH2	1:B:274:ASP:OD1	2.47	0.46
1:B:268:ARG:NE	2:B:441:HOH:O	2.48	0.46
1:A:68:ILE:HD11	1:A:258:PHE:CD2	2.50	0.46
1:D:89:THR:CG2	1:D:216:GLU:OE2	2.60	0.46
1:C:242:ASN:O	2:C:448:HOH:O	2.19	0.46
1:B:116:LEU:HA	1:B:145:ILE:HG22	1.98	0.46
1:A:78:ASN:OD1	1:D:74:ASP:HB3	2.16	0.45
1:B:179:GLU:OE2	1:B:211:ARG:NE	2.49	0.45
1:D:52:VAL:HG23	1:D:84:LEU:HD21	1.97	0.45
1:A:61:HIS:O	1:A:64:ARG:HD3	2.17	0.45
1:A:114:TYR:CD1	1:A:262:LEU:HD11	2.52	0.45
1:A:182:ILE:HG22	1:A:186:ILE:CD1	2.47	0.45
1:C:241:LEU:HD21	1:C:245:ARG:CZ	2.47	0.45
1:B:102:LYS:NZ	2:B:422:HOH:O	1.92	0.45
1:C:132:CYS:O	1:C:135:LEU:HB2	2.17	0.45
1:D:83:ALA:HA	1:D:217:LEU:HD11	1.98	0.45
1:D:182:ILE:HG22	1:D:186:ILE:CD1	2.46	0.45
1:B:131:THR:CG2	1:B:134:GLU:OE1	2.45	0.44
1:C:243:ALA:C	2:C:448:HOH:O	2.34	0.44
1:D:262:LEU:HD12	1:D:262:LEU:HA	1.80	0.44
1:C:97:GLY:HA2	1:C:102:LYS:HG2	1.99	0.44
1:C:130:LEU:HB3	1:C:259:PHE:CD1	2.52	0.44
1:C:173:GLU:HB3	1:C:239:ARG:HG3	1.98	0.44
1:B:179:GLU:HG3	1:B:214:ALA:HB2	2.00	0.44
1:B:113:GLU:CB	1:B:148:ILE:HD12	2.48	0.44
1:B:130:LEU:HD23	1:B:130:LEU:HA	1.82	0.44
1:C:87:SER:O	1:C:91:ARG:HG3	2.17	0.44
1:A:168:ASP:OD1	1:A:250:ARG:HD3	2.18	0.44
1:B:146:PHE:CB	1:B:147:PRO:CD	2.95	0.44
1:B:236:LEU:HD22	1:B:236:LEU:HA	1.80	0.44
1:C:257:ALA:HA	1:C:260:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:LYS:HE3	1:C:102:LYS:HB3	1.55	0.43
1:D:154:ASN:OD1	1:D:157:GLU:N	2.52	0.43
1:D:249:MSE:HE2	2:D:410:HOH:O	2.18	0.43
1:B:72:THR:O	1:B:76:ILE:HG13	2.18	0.43
1:D:242:ASN:ND2	1:D:242:ASN:H	2.16	0.43
1:C:83:ALA:HA	1:C:217:LEU:HD11	2.01	0.43
1:C:246:GLN:O	1:C:250:ARG:HB2	2.19	0.43
1:D:68:ILE:HD13	1:D:68:ILE:C	2.38	0.43
1:C:66:ARG:HA	1:C:265:ILE:HG12	2.00	0.43
1:C:68:ILE:HD12	1:C:262:LEU:HD13	2.01	0.43
1:C:133:ASN:CG	2:C:468:HOH:O	2.55	0.43
1:C:132:CYS:SG	1:C:248:ALA:HB1	2.59	0.42
1:D:209:LEU:O	1:D:213:VAL:HG23	2.19	0.42
1:A:143:GLU:HA	1:A:144:PRO:HD3	1.82	0.42
1:A:174:MSE:O	1:A:178:GLN:HG3	2.18	0.42
1:C:64:ARG:NH2	1:C:274:ASP:OD1	2.52	0.42
1:B:58:ARG:HG2	2:C:416:HOH:O	2.19	0.42
1:A:221:VAL:CB	2:A:467:HOH:O	2.66	0.42
1:D:182:ILE:O	1:D:186:ILE:HD12	2.20	0.42
1:D:211:ARG:HD3	1:D:211:ARG:HA	1.62	0.42
1:A:82:ASP:OD1	1:A:86:ARG:HD3	2.20	0.42
1:A:116:LEU:O	1:A:118:GLU:OE1	2.37	0.42
1:A:231:GLU:H	1:A:231:GLU:HG2	1.48	0.42
1:A:257:ALA:HB1	1:A:277:GLU:HG3	2.02	0.42
1:B:169:THR:HA	1:B:174:MSE:HE3	2.01	0.42
1:D:114:TYR:HA	1:D:147:PRO:HA	2.01	0.42
1:D:115:GLU:HB2	2:D:432:HOH:O	2.19	0.42
1:A:53:TYR:CZ	1:D:54:GLU:HG3	2.55	0.42
1:C:105:ILE:H	1:C:105:ILE:HG13	1.62	0.42
1:D:242:ASN:HA	1:D:245:ARG:HB2	2.01	0.41
2:B:404:HOH:O	1:C:58:ARG:HG3	2.20	0.41
1:D:89:THR:HG23	1:D:216:GLU:CD	2.40	0.41
1:D:131:THR:HG22	1:D:134:GLU:HG3	2.00	0.41
1:B:68:ILE:HD12	1:B:258:PHE:CE2	2.55	0.41
1:D:131:THR:CG2	1:D:134:GLU:CG	2.92	0.41
1:A:79:THR:HG21	1:A:177:TRP:HZ3	1.85	0.41
1:D:68:ILE:HG21	1:D:165:VAL:CG1	2.49	0.41
1:C:204:GLY:N	1:C:205:PRO:CD	2.84	0.41
1:B:98:ILE:HG22	1:B:99:HIS:ND1	2.36	0.41
1:D:86:ARG:HB2	1:D:217:LEU:CD2	2.50	0.41
1:D:232:ARG:O	1:D:236:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:MSE:HA	1:B:249:MSE:CE	2.50	0.41
1:C:56:VAL:O	1:C:60:VAL:HG23	2.21	0.41
1:A:145:ILE:O	1:A:145:ILE:HG13	2.21	0.40
1:B:140:VAL:O	1:B:142:GLN:HG2	2.21	0.40
1:C:233:GLU:OE2	1:C:237:ARG:HD2	2.21	0.40
1:C:257:ALA:O	1:C:261:ARG:N	2.31	0.40
1:A:83:ALA:HA	1:A:217:LEU:HD11	2.03	0.40
1:A:182:ILE:HG21	1:A:213:VAL:HG11	2.02	0.40
1:A:100:ASN:O	1:A:101:GLU:HB2	2.20	0.40
1:C:87:SER:HB2	1:C:217:LEU:HD21	2.02	0.40
1:C:151:ALA:HB1	1:C:188:HIS:CD2	2.56	0.40
1:D:79:THR:HG21	1:D:177:TRP:HZ3	1.85	0.40
1:D:179:GLU:OE2	1:D:211:ARG:NE	2.38	0.40
1:C:126:ASP:OD2	1:C:128:GLN:CB	2.68	0.40
1:D:247:ALA:O	1:D:250:ARG:HB2	2.22	0.40
1:C:79:THR:HG21	1:C:177:TRP:HZ3	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASP:OD2	2:D:430:HOH:O[2_556]	1.94	0.26

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	206/264 (78%)	200 (97%)	5 (2%)	1 (0%)	25	32
1	B	196/264 (74%)	190 (97%)	6 (3%)	0	100	100
1	C	200/264 (76%)	193 (96%)	6 (3%)	1 (0%)	25	32
1	D	196/264 (74%)	184 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	798/1056 (76%)	767 (96%)	29 (4%)	2 (0%)	37	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	GLU
1	A	164	SER

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	175/228 (77%)	156 (89%)	19 (11%)	5	6
1	B	174/228 (76%)	157 (90%)	17 (10%)	6	8
1	C	171/228 (75%)	158 (92%)	13 (8%)	11	14
1	D	167/228 (73%)	145 (87%)	22 (13%)	3	3
All	All	687/912 (75%)	616 (90%)	71 (10%)	6	7

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	55	SER
1	A	68	ILE
1	A	105	ILE
1	A	118	GLU
1	A	128	GLN
1	A	131	THR
1	A	135	LEU
1	A	139	ASP
1	A	146	PHE
1	A	212	ARG
1	A	215	GLN
1	A	220	SER

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Mol	Chain	Res	Type
1	A	231	GLU
1	A	237	ARG
1	A	238	LEU
1	A	244	LEU
1	A	249	MSE
1	A	260	GLU
1	B	52	VAL
1	B	68	ILE
1	B	89	THR
1	B	95	SER
1	B	99	HIS
1	B	118	GLU
1	B	128	GLN
1	B	132	CYS
1	B	138	TYR
1	B	146	PHE
1	B	192	SER
1	B	212	ARG
1	B	215	GLN
1	B	236	LEU
1	B	238	LEU
1	B	244	LEU
1	B	249	MSE
1	C	64	ARG
1	C	68	ILE
1	C	79	THR
1	C	102	LYS
1	C	105	ILE
1	C	132	CYS
1	C	139	ASP
1	C	146	PHE
1	C	192	SER
1	C	212	ARG
1	C	233	GLU
1	C	244	LEU
1	C	268	ARG
1	D	52	VAL
1	D	62	ASP
1	D	68	ILE
1	D	79	THR
1	D	89	THR
1	D	105	ILE

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Mol	Chain	Res	Type
1	D	118	GLU
1	D	119	GLU
1	D	121	SER
1	D	128	GLN
1	D	129	SER
1	D	132	CYS
1	D	143	GLU
1	D	146	PHE
1	D	149	CYS
1	D	173	GLU
1	D	192	SER
1	D	211	ARG
1	D	215	GLN
1	D	236	LEU
1	D	238	LEU
1	D	268	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	178	GLN
1	B	71	HIS
1	B	142	GLN
1	D	242	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	209/264 (79%)	0.69	23 (11%)	12 13	21, 37, 72, 106	0
1	B	203/264 (76%)	0.62	20 (9%)	14 16	20, 36, 69, 89	0
1	C	205/264 (77%)	0.82	28 (13%)	8 9	20, 38, 76, 112	0
1	D	203/264 (76%)	1.19	38 (18%)	4 5	22, 49, 86, 113	0
All	All	820/1056 (77%)	0.83	109 (13%)	8 9	20, 39, 79, 113	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	193	SER	7.5
1	B	50	SER	6.9
1	D	124	ILE	6.7
1	A	221	VAL	6.7
1	A	50	SER	6.4
1	C	193	SER	5.9
1	A	51	ASN	5.7
1	A	193	SER	5.6
1	A	230	PRO	5.5
1	B	122	VAL	5.0
1	A	138	TYR	5.0
1	C	138	TYR	4.8
1	D	125	ASP	4.8
1	D	231	GLU	4.7
1	C	50	SER	4.5
1	C	124	ILE	4.5
1	D	129	SER	4.3
1	D	50	SER	4.2
1	D	132	CYS	4.1
1	C	118	GLU	4.1
1	C	122	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	220	SER	3.9
1	C	121	SER	3.7
1	D	116	LEU	3.7
1	C	132	CYS	3.7
1	D	127	ILE	3.5
1	D	256	ARG	3.5
1	D	142	GLN	3.4
1	A	122	VAL	3.4
1	B	126	ASP	3.4
1	B	232	ARG	3.4
1	D	118	GLU	3.4
1	D	137	GLU	3.2
1	D	130	LEU	3.2
1	C	136	TYR	3.2
1	B	140	VAL	3.2
1	A	268	ARG	3.1
1	C	51	ASN	3.1
1	A	118	GLU	3.1
1	B	124	ILE	3.0
1	C	203	LEU	3.0
1	B	220	SER	3.0
1	C	129	SER	2.9
1	C	149	CYS	2.8
1	D	149	CYS	2.8
1	A	203	LEU	2.8
1	C	155	ASP	2.8
1	D	126	ASP	2.8
1	A	149	CYS	2.8
1	D	203	LEU	2.8
1	A	101	GLU	2.7
1	D	278	TYR	2.7
1	C	99	HIS	2.7
1	D	253	GLU	2.6
1	B	132	CYS	2.6
1	D	146	PHE	2.6
1	D	95	SER	2.6
1	D	236	LEU	2.6
1	C	191	GLY	2.6
1	D	148	ILE	2.6
1	D	265	ILE	2.6
1	B	149	CYS	2.6
1	B	192	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	121	SER	2.5
1	B	118	GLU	2.5
1	A	135	LEU	2.5
1	C	232	ARG	2.5
1	A	211	ARG	2.5
1	D	218	GLY	2.5
1	D	99	HIS	2.5
1	A	132	CYS	2.4
1	A	130	LEU	2.4
1	B	152	GLY	2.4
1	B	252	GLU	2.4
1	D	232	ARG	2.4
1	D	122	VAL	2.3
1	B	203	LEU	2.3
1	C	253	GLU	2.3
1	D	239	ARG	2.3
1	D	160	TYR	2.3
1	A	233	GLU	2.3
1	A	156	ASN	2.3
1	C	105	ILE	2.3
1	C	79	THR	2.2
1	D	55	SER	2.2
1	C	115	GLU	2.2
1	B	51	ASN	2.2
1	A	68	ILE	2.2
1	D	244	LEU	2.2
1	D	117	ASN	2.1
1	D	144	PRO	2.1
1	B	215	GLN	2.1
1	D	248	ALA	2.1
1	C	139	ASP	2.1
1	A	124	ILE	2.1
1	C	135	LEU	2.1
1	C	142	GLN	2.1
1	C	156	ASN	2.1
1	A	248	ALA	2.1
1	B	137	GLU	2.0
1	D	120	SER	2.0
1	B	235	HIS	2.0
1	C	241	LEU	2.0
1	A	260	GLU	2.0
1	C	137	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	187	HIS	2.0
1	A	121	SER	2.0
1	C	265	ILE	2.0
1	B	128	GLN	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.