



# Full wwPDB X-ray Structure Validation Report i

May 13, 2020 – 12:44 pm BST

PDB ID : 4LGI  
Title : N-terminal truncated NleC structure  
Authors : Li, W.Q.; Liu, Y.X.; Sheng, X.L.; Yan, C.Y.; Wang, J.W.  
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](mailto: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.

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The following versions of software and data (see [references](#) ①) 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 : 2.11  
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

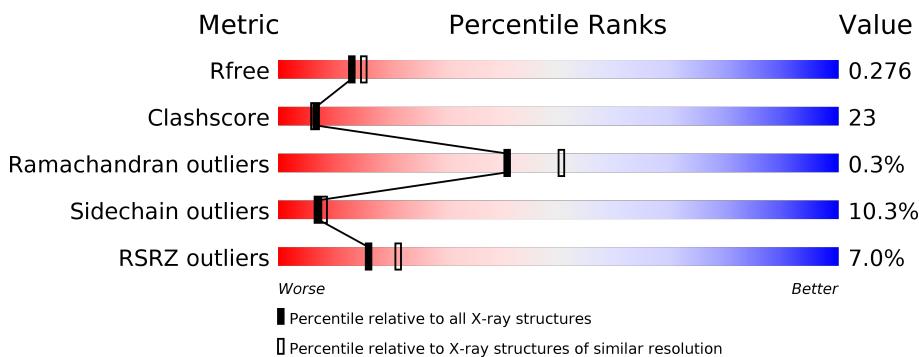
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

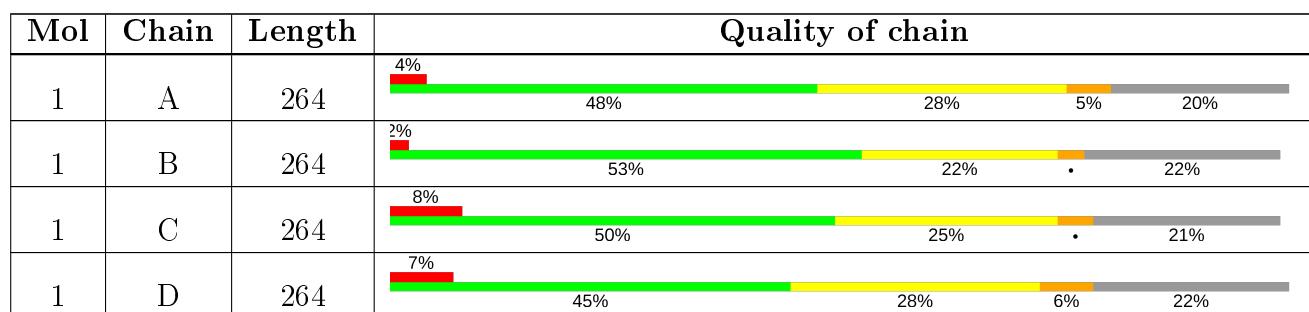
The reported resolution of this entry is 2.30 Å.

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.



## 2 Entry composition i

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			

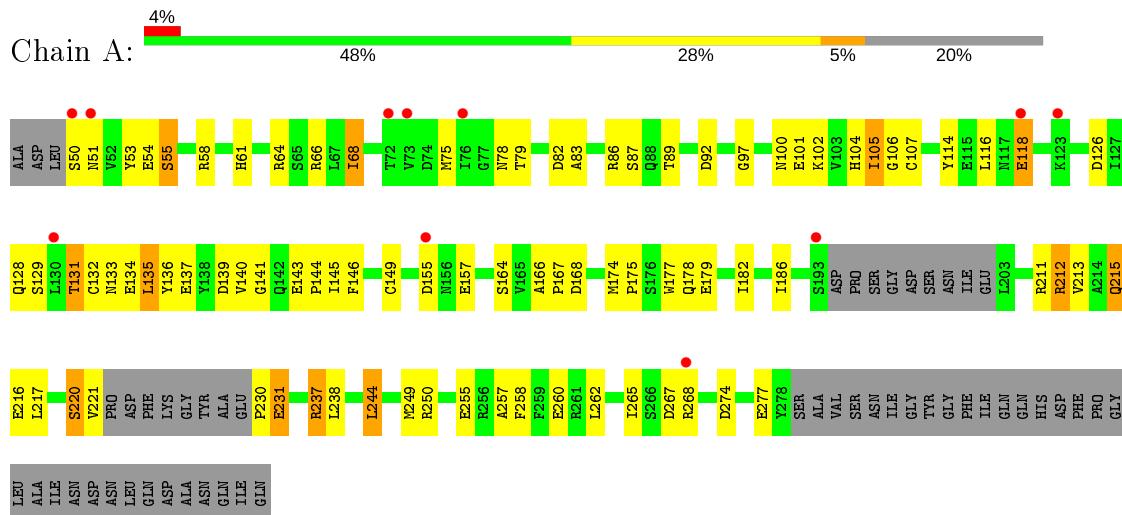
- Molecule 2 is water.

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

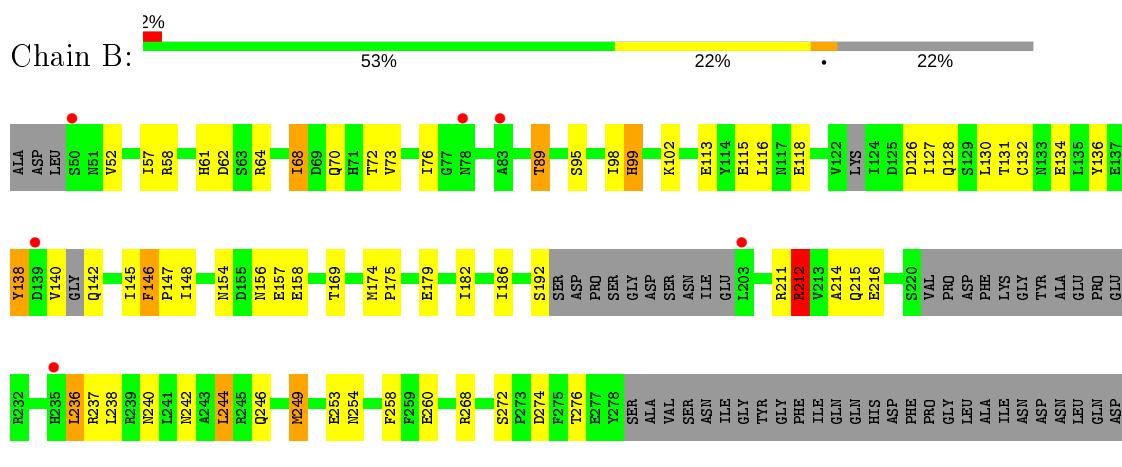
### 3 Residue-property plots

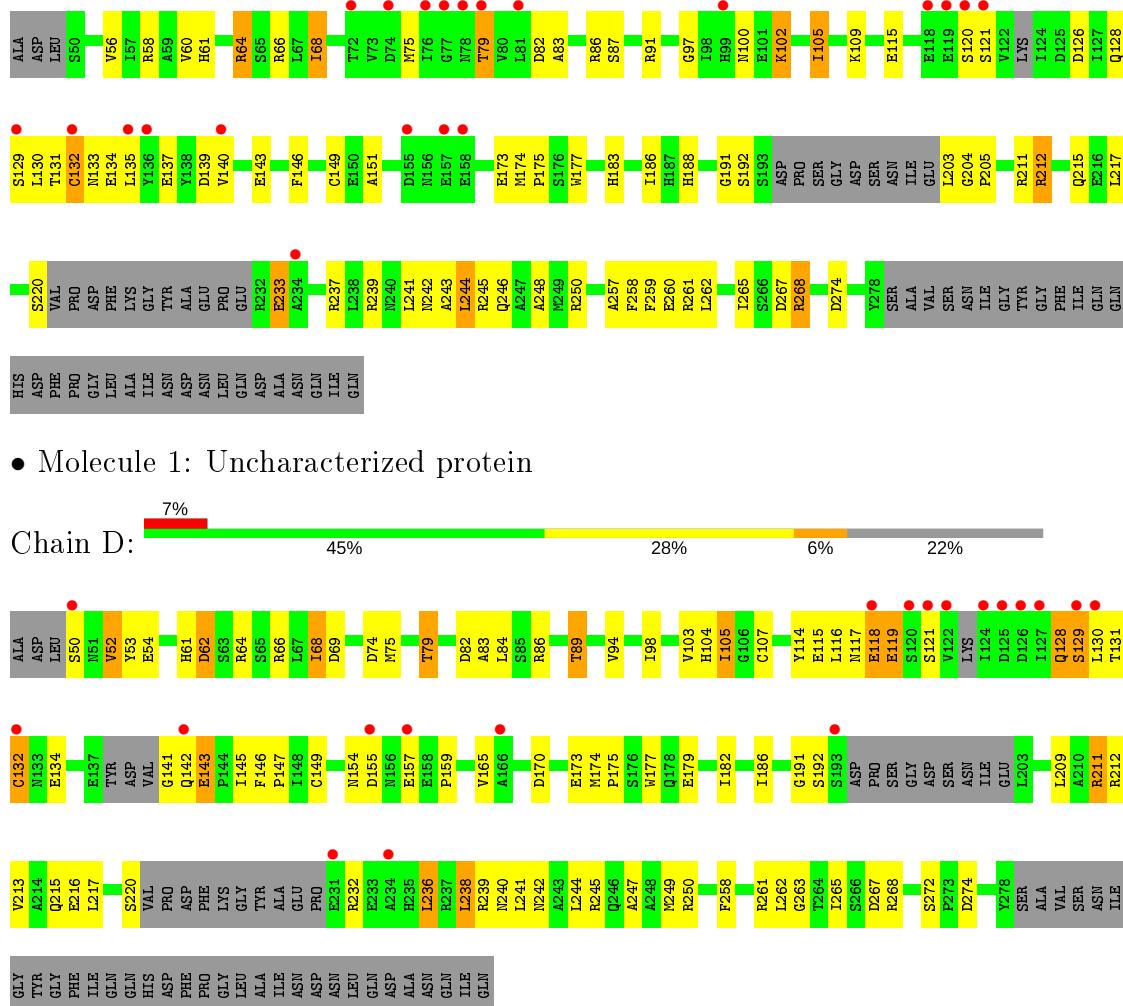
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



- Molecule 1: Uncharacterized protein





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.51 Å    88.66 Å    110.65 Å 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) 99.5 (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 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
$R$ , $R_{free}$	0.253 , 0.280 0.247 , 0.276	Depositor DCC
$R_{free}$ test set	2571 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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( $^{\circ}$ )	Ideal( $^{\circ}$ )
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:NH1	1:C:212:ARG:HG3	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:OE1	1:A:118:GLU:N	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:131:THR:HG23	1:A:134:GLU:CG	2.41	0.51
1:A:89:THR:HB	2:A:454:HOH:O	2.07	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:114:TYR:CZ	1:D:147:PRO:HB3	2.46	0.50
1:D:52:VAL:CG1	2:D:413:HOH:O	2.58	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:104:HIS:HB3	1:D:107:CYS:SG	2.52	0.49
1:D:61:HIS:O	1:D:64:ARG:HD3	2.12	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:104:HIS:O	1:A:107:CYS:HB2	2.13	0.48
1:A:68:ILE:HD12	1:A:258:PHE:CE2	2.49	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:268:ARG:NE	2:B:441:HOH:O	2.48	0.46
1:B:64:ARG:NH2	1:B:274:ASP:OD1	2.47	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:114:TYR:CD1	1:A:262:LEU:HD11	2.52	0.45
1:A:61:HIS:O	1:A:64:ARG:HD3	2.17	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:182:ILE:HG22	1:D:186:ILE:CD1	2.46	0.45
1:D:83:ALA:HA	1:D:217:LEU:HD11	1.98	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:173:GLU:HB3	1:C:239:ARG:HG3	1.98	0.44
1:C:130:LEU:HB3	1:C:259:PHE:CD1	2.52	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:HA	1:B:130:LEU:HD23	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:HA	1:B:236:LEU:HD22	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:246:GLN:O	1:C:250:ARG:HB2	2.19	0.43
1:C:83:ALA:HA	1:C:217:LEU:HD11	2.01	0.43
1:D:68:ILE:C	1:D:68:ILE:HD13	2.38	0.43
1:C:66:ARG:HA	1:C:265:ILE:HG12	2.00	0.43
1:C:133:ASN:CG	2:C:468:HOH:O	2.55	0.43
1:C:68:ILE:HD12	1:C:262:LEU:HD13	2.01	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: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:82:ASP:OD1	1:A:86:ARG:HD3	2.20	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:115:GLU:HB2	2:D:432:HOH:O	2.19	0.42
1:D:114:TYR:HA	1:D:147:PRO:HA	2.01	0.42
1:C:105:ILE:HG13	1:C:105:ILE:H	1.62	0.42
1:A:53:TYR:CZ	1:D:54:GLU:HG3	2.55	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:131:THR:HG22	1:D:134:GLU:HG3	2.00	0.41
1:D:89:THR:HG23	1:D:216:GLU:CD	2.40	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:182:ILE:HG21	1:A:213:VAL:HG11	2.02	0.40
1:A:83:ALA:HA	1:A:217:LEU:HD11	2.03	0.40
1:A:100:ASN:O	1:A:101:GLU:HB2	2.20	0.40
1:C:151:ALA:HB1	1:C:188:HIS:CD2	2.56	0.40
1:C:87:SER:HB2	1:C:217:LEU:HD21	2.02	0.40
1:D:179:GLU:OE2	1:D:211:ARG:NE	2.38	0.40
1:D:79:THR:HG21	1:D:177:TRP:HZ3	1.85	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 [\(i\)](#)

### 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	206/264 (78%)	200 (97%)	5 (2%)	1 (0%)	29 35
1	B	196/264 (74%)	190 (97%)	6 (3%)	0	100 100
1	C	200/264 (76%)	193 (96%)	6 (3%)	1 (0%)	29 35
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%)	41 50

All (2) Ramachandran outliers are listed below:

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

### 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	175/228 (77%)	156 (89%)	19 (11%)	6 7
1	B	174/228 (76%)	157 (90%)	17 (10%)	8 9
1	C	171/228 (75%)	158 (92%)	13 (8%)	13 16
1	D	167/228 (73%)	145 (87%)	22 (13%)	4 4
All	All	687/912 (75%)	616 (90%)	71 (10%)	7 8

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

Some 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 [\(i\)](#)

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 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	209/264 (79%)	0.36	11 (5%) 26 33	21, 37, 72, 106	0
1	B	203/264 (76%)	0.32	6 (2%) 50 57	20, 36, 69, 89	0
1	C	205/264 (77%)	0.53	21 (10%) 6 9	20, 38, 76, 112	0
1	D	203/264 (76%)	0.63	19 (9%) 8 11	22, 49, 86, 113	0
All	All	820/1056 (77%)	0.46	57 (6%) 16 21	20, 39, 79, 113	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	ILE	6.2
1	D	193	SER	6.1
1	D	50	SER	5.1
1	A	193	SER	5.0
1	C	121	SER	5.0
1	D	234	ALA	4.7
1	D	125	ASP	4.5
1	A	50	SER	3.8
1	A	76	ILE	3.6
1	D	129	SER	3.5
1	D	127	ILE	3.5
1	D	132	CYS	3.4
1	A	51	ASN	3.3
1	C	140	VAL	3.3
1	D	118	GLU	3.1
1	C	132	CYS	3.1
1	C	157	GLU	3.0
1	B	78	ASN	3.0
1	C	76	ILE	3.0
1	D	126	ASP	3.0
1	C	79	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	155	ASP	2.9
1	D	157	GLU	2.9
1	B	235	HIS	2.9
1	B	203	LEU	2.8
1	D	130	LEU	2.8
1	C	81	LEU	2.7
1	D	142	GLN	2.7
1	C	234	ALA	2.7
1	A	72	THR	2.7
1	D	231	GLU	2.6
1	A	155	ASP	2.6
1	C	74	ASP	2.6
1	C	118	GLU	2.5
1	C	77	GLY	2.5
1	C	78	ASN	2.5
1	D	122	VAL	2.5
1	D	120	SER	2.4
1	A	130	LEU	2.4
1	D	166	ALA	2.4
1	C	72	THR	2.3
1	D	155	ASP	2.3
1	A	268	ARG	2.3
1	D	121	SER	2.3
1	B	139	ASP	2.3
1	C	158	GLU	2.2
1	A	73	VAL	2.2
1	B	50	SER	2.2
1	C	129	SER	2.2
1	C	120	SER	2.2
1	A	123	LYS	2.1
1	C	136	TYR	2.1
1	C	135	LEU	2.1
1	A	118	GLU	2.1
1	B	83	ALA	2.1
1	C	99	HIS	2.0
1	C	119	GLU	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.