W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:24 PM GMT

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

A user guide is available at

http://wwpdb.org/validation/2016/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	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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	Percentile Ranks	Value
Rfree		0.280
Clashscore		23
Ramachandran outliers		0.3%
Sidechain outliers		10.3%
RSRZ outliers		7.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
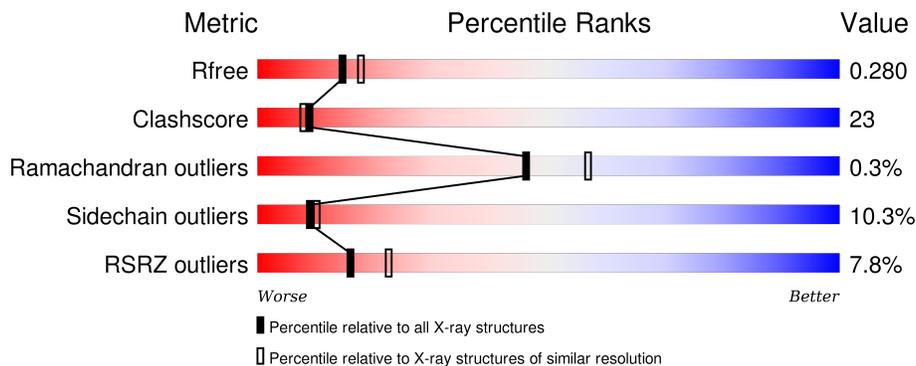
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	264	4% / 48% 28% 5% 20%
1	B	264	3% / 53% 22% • 22%
1	C	264	9% / 50% 25% • 21%
1	D	264	8% / 45% 28% 6% 22%

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	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
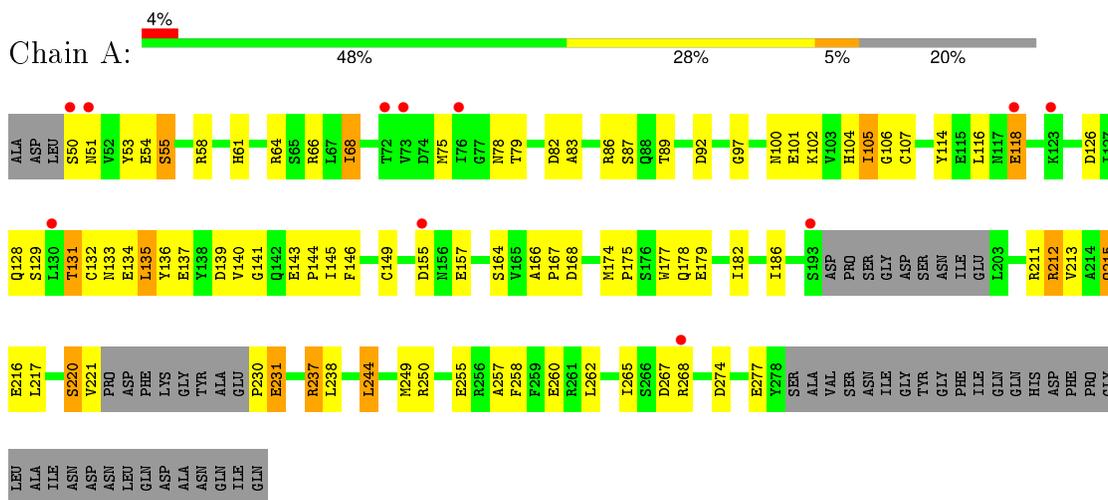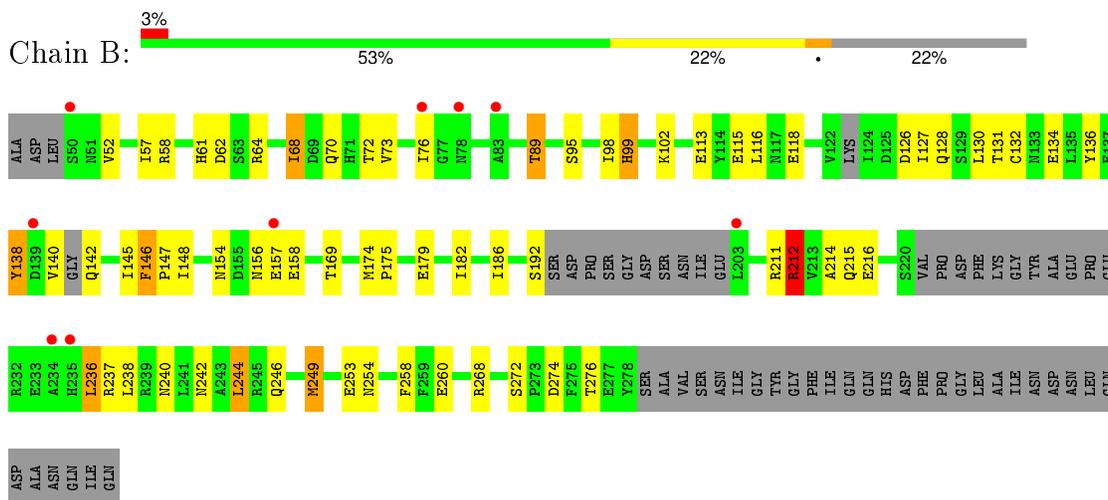
- Molecule 1: Uncharacterized protein

- Molecule 1: Uncharacterized protein

• Molecule 1: Uncharacterized protein

Chain D:
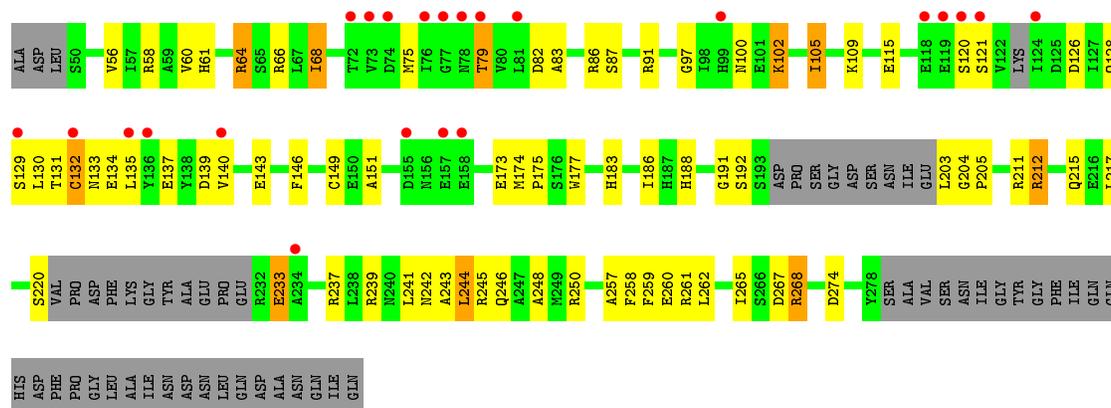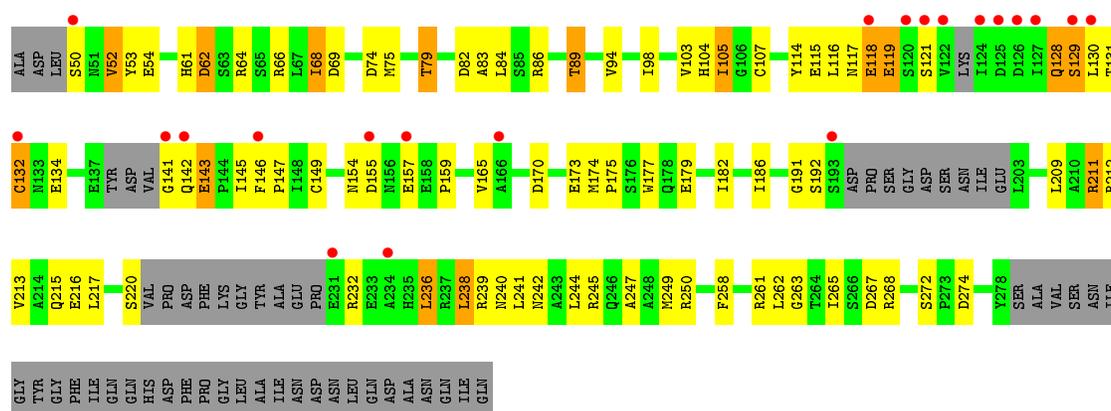
4   Data and refinement statistics (i)

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) 99.5 (37.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.59 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.253 , 0.280 0.251 , 0.280	Depositor DCC
R_{free} test set	2571 reflections (5.33%)	DCC
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 , 36.4	EDS
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.47$, $<L^2> = 0.30$	Xtriage
Outliers	0 of 50831 reflections	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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:D:52:VAL:N	2:D:413:HOH:O	1.82	1.07
1:A:157:GLU:HB3	2:A:468:HOH:O	1.53	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: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:C:241:LEU:O	2:C:448:HOH:O	1.90	0.88
1:B:89:THR:CG2	1:B:216:GLU:OE2	2.21	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:89:THR:HG22	1:B:216:GLU:CD	2.06	0.75
1:B:62:ASP:OD1	2:B:423:HOH:O	2.05	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:C:102:LYS:HE2	1:C:191:GLY:HA3	1.82	0.60
1:A:135:LEU:HD21	1:A:244:LEU:HD13	1.84	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:D:66:ARG:HG3	2:D:431:HOH:O	2.00	0.57
1:C:211:ARG:O	1:C:215:GLN:HG3	2.03	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:D:238:LEU:HG	1:D:242:ASN:HD21	1.76	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: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:D:68:ILE:HD11	1:D:258:PHE:CD1	2.46	0.50
1:A:104:HIS:HB3	1:A:107:CYS:SG	2.51	0.50
1:D:75:MSE:O	1:D:79:THR:CG2	2.51	0.50
1:A:211:ARG:NH1	2:A:467:HOH:O	2.00	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:D:174:MSE:HB3	1:D:175:PRO:HD3	1.94	0.48
1:B:136:TYR:N	1:B:136:TYR:CD1	2.81	0.48
1:D:50:SER:HA	1:D:53:TYR:CD2	2.34	0.48
1:D:66:ARG:C	1:D:265:ILE:HD13	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: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:D:145:ILE:HD11	1:D:244:LEU:HD11	1.96	0.47
1:A:182:ILE:HG22	1:A:186:ILE:HD11	1.96	0.47
1:D:75:MSE:HG3	1:D:174:MSE:HE1	1.95	0.47
1:C:174:MSE:HB3	1:C:175:PRO:HD3	1.95	0.47
1:D:241:LEU:CD2	1:D:245:ARG:NH1	2.77	0.47
1:D:191:GLY:HA2	2:D:412:HOH:O	2.15	0.47
1:B:182:ILE:O	1:B:186:ILE:HG13	2.15	0.47
1:D:239:ARG:NH2	1:D:240:ASN:OD1	2.29	0.47
1:A:136:TYR:N	1:A:136:TYR:CD1	2.81	0.47
1:C:120:SER:OG	1:C:121:SER:N	2.48	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:D:89:THR:CG2	1:D:216:GLU:OE2	2.60	0.46
1:A:68:ILE:HD11	1:A:258:PHE:CD2	2.50	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:C:241:LEU:HD21	1:C:245:ARG:CZ	2.47	0.45
1:A:182:ILE:HG22	1:A:186:ILE:CD1	2.47	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: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: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:130:LEU:HA	1:B:130:LEU:HD23	1.82	0.44
1:B:113:GLU:CB	1:B:148:ILE:HD12	2.48	0.44
1:C:87:SER:O	1:C:91:ARG:HG3	2.17	0.44
1:B:236:LEU:HA	1:B:236:LEU:HD22	1.80	0.44
1:B:146:PHE:CB	1:B:147:PRO:CD	2.95	0.44
1:A:168:ASP:OD1	1:A:250:ARG:HD3	2.18	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:D:242:ASN:ND2	1:D:242:ASN:H	2.16	0.43
1:B:72:THR:O	1:B:76:ILE:HG13	2.18	0.43
1:C:246:GLN:O	1:C:250:ARG:HB2	2.19	0.43
1:D:68:ILE:C	1:D:68:ILE:HD13	2.38	0.43
1:C:83:ALA:HA	1:C:217:LEU:HD11	2.01	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: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:A:143:GLU:HA	1:A:144:PRO:HD3	1.82	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:82:ASP:OD1	1:A:86:ARG:HD3	2.20	0.42
1:A:231:GLU:H	1:A:231:GLU:HG2	1.48	0.42
1:B:169:THR:HA	1:B:174:MSE:HE3	2.01	0.42
1:A:257:ALA:HB1	1:A:277:GLU:HG3	2.02	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:A:53:TYR:CZ	1:D:54:GLU:HG3	2.55	0.42
1:C:105:ILE:HG13	1:C:105:ILE:H	1.62	0.42
1:D:242:ASN:HA	1:D:245:ARG:HB2	2.01	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
2:B:404:HOH:O	1:C:58:ARG:HG3	2.20	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:D:86:ARG:HB2	1:D:217:LEU:CD2	2.50	0.41
1:B:98:ILE:HG22	1:B:99:HIS:ND1	2.36	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:257:ALA:O	1:C:261:ARG:N	2.31	0.40
1:C:233:GLU:OE2	1:C:237:ARG:HD2	2.21	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:D:79:THR:HG21	1:D:177:TRP:HZ3	1.85	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: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: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%)	34	41
1	B	196/264 (74%)	190 (97%)	6 (3%)	0	100	100
1	C	200/264 (76%)	193 (96%)	6 (3%)	1 (0%)	34	41
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%)	46 57

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%)	8 9
1	B	174/228 (76%)	157 (90%)	17 (10%)	10 11
1	C	171/228 (75%)	158 (92%)	13 (8%)	16 20
1	D	167/228 (73%)	145 (87%)	22 (13%)	5 5
All	All	687/912 (75%)	616 (90%)	71 (10%)	9 10

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, 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(Å²)	Q<0.9
1	A	209/264 (79%)	0.43	11 (5%)	30	39	21, 37, 72, 106	0
1	B	203/264 (76%)	0.39	9 (4%)	38	47	20, 36, 69, 89	0
1	C	205/264 (77%)	0.60	23 (11%)	7	10	20, 38, 76, 112	0
1	D	203/264 (76%)	0.71	21 (10%)	9	13	22, 49, 86, 113	0
All	All	820/1056 (77%)	0.53	64 (7%)	16	22	20, 39, 79, 113	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	ILE	6.3
1	D	193	SER	6.2
1	D	50	SER	5.4
1	A	193	SER	5.3
1	C	121	SER	5.2
1	D	234	ALA	5.0
1	D	125	ASP	4.7
1	A	50	SER	4.1
1	A	76	ILE	3.7
1	D	127	ILE	3.6
1	D	132	CYS	3.6
1	D	129	SER	3.5
1	A	51	ASN	3.4
1	C	140	VAL	3.4
1	D	118	GLU	3.2
1	C	132	CYS	3.1
1	C	76	ILE	3.1
1	C	157	GLU	3.1
1	C	155	ASP	3.1
1	C	79	THR	3.1
1	B	235	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	126	ASP	3.1
1	B	78	ASN	3.0
1	D	157	GLU	3.0
1	B	203	LEU	3.0
1	C	81	LEU	2.9
1	C	234	ALA	2.8
1	D	130	LEU	2.8
1	D	142	GLN	2.8
1	A	72	THR	2.8
1	A	155	ASP	2.7
1	D	122	VAL	2.7
1	C	74	ASP	2.7
1	C	77	GLY	2.6
1	D	231	GLU	2.6
1	C	118	GLU	2.6
1	C	78	ASN	2.6
1	A	130	LEU	2.6
1	D	120	SER	2.5
1	D	166	ALA	2.5
1	C	72	THR	2.5
1	D	155	ASP	2.4
1	A	73	VAL	2.4
1	B	50	SER	2.4
1	B	139	ASP	2.4
1	C	158	GLU	2.3
1	C	129	SER	2.3
1	A	268	ARG	2.3
1	C	135	LEU	2.3
1	C	120	SER	2.3
1	B	83	ALA	2.3
1	D	121	SER	2.2
1	A	118	GLU	2.2
1	C	136	TYR	2.2
1	B	157	GLU	2.1
1	C	99	HIS	2.1
1	A	123	LYS	2.1
1	C	119	GLU	2.1
1	C	124	ILE	2.1
1	D	141	GLY	2.1
1	C	73	VAL	2.1
1	B	76	ILE	2.1
1	D	146	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	234	ALA	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.