



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:43 pm BST

PDB ID : 3KLN  
Title : Vibrio cholerae VpsT  
Authors : Krasteva, P.V.; Navarro, V.A.S.; Sondermann, H.  
Deposited on : 2009-11-08  
Resolution : 3.08 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 ⓘ symbol.

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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

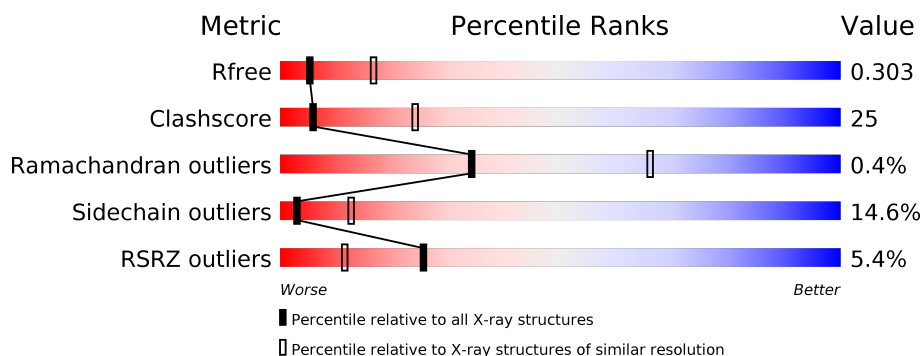
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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.

Mol	Chain	Length	Quality of chain
1	A	225	<div> <div>55%</div> <div>34%</div> <div>8%</div> <div>•</div> </div>
1	B	225	<div> <div>%</div> <div>52%</div> <div>35%</div> <div>9%</div> <div>•</div> </div>
1	C	225	<div> <div>6%</div> <div>52%</div> <div>34%</div> <div>8%</div> <div>5%</div> </div>
1	D	225	<div> <div>12%</div> <div>41%</div> <div>30%</div> <div>6%</div> <div>23%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6640 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 Transcriptional regulator, LuxR family.

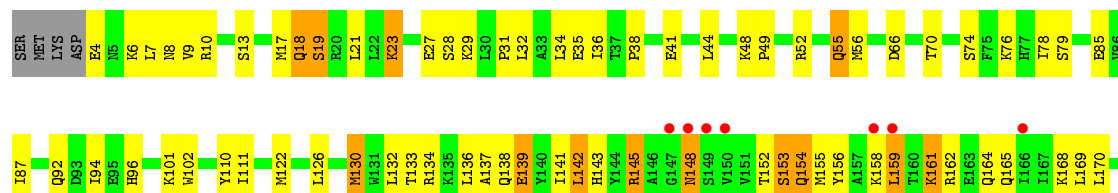
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1756	1119	298	329	10			
1	B	215	Total	C	N	O	S	0	0	0
			1739	1110	296	323	10			
1	C	213	Total	C	N	O	S	0	0	0
			1728	1101	294	323	10			
1	D	173	Total	C	N	O	S	0	0	0
			1417	905	241	262	9			

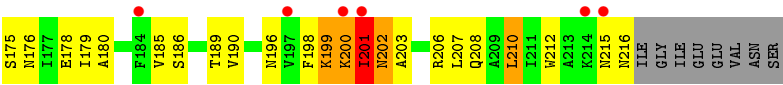
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q9KKZ8
B	0	SER	-	EXPRESSION TAG	UNP Q9KKZ8
C	0	SER	-	EXPRESSION TAG	UNP Q9KKZ8
D	0	SER	-	EXPRESSION TAG	UNP Q9KKZ8

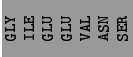
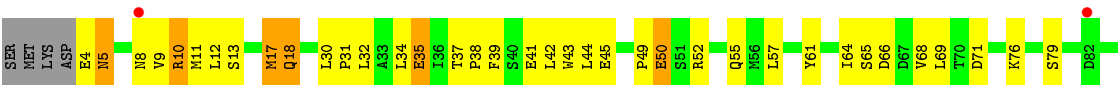
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:  55% 34% 8% 3%





● Molecule 1: Transcriptional regulator, LuxR family



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.49 Å   121.49 Å   198.29 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	45.90 – 3.08 47.65 – 3.08	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.90-3.08) 99.1 (47.65-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.07 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.247   ,   0.308 0.251   ,   0.303	Depositor DCC
$R_{free}$ test set	1400 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.3	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1867e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.64	0/1785	0.68	0/2407
1	B	0.58	0/1768	0.64	0/2384
1	C	0.42	0/1757	0.59	0/2369
1	D	0.44	0/1443	0.60	0/1947
All	All	0.53	0/6753	0.63	0/9107

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	1756	0	1796	78	0
1	B	1739	0	1786	104	0
1	C	1728	0	1767	81	0
1	D	1417	0	1435	81	0
All	All	6640	0	6784	337	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 25.

All (337) 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:B:145:ARG:HH11	1:B:145:ARG:HG2	1.04	1.16
1:D:143:HIS:CE1	1:D:148:ASN:HB2	1.91	1.05
1:A:130:MET:CE	1:A:132:LEU:HD11	1.91	0.99
1:D:18:GLN:NE2	1:D:18:GLN:H	1.61	0.99
1:A:130:MET:HE2	1:A:132:LEU:HD11	1.01	0.98
1:D:18:GLN:N	1:D:18:GLN:HE21	1.61	0.98
1:B:130:MET:HE1	1:B:132:LEU:HD11	1.44	0.97
1:B:18:GLN:HE21	1:B:18:GLN:N	1.63	0.96
1:B:18:GLN:NE2	1:B:18:GLN:H	1.63	0.96
1:C:18:GLN:HE21	1:C:18:GLN:H	0.95	0.94
1:B:201:ILE:O	1:B:202:ASN:HB3	1.71	0.91
1:B:130:MET:CE	1:B:132:LEU:HD11	2.01	0.90
1:A:18:GLN:HE21	1:A:18:GLN:H	1.10	0.90
1:B:186:SER:HB3	1:B:189:THR:OG1	1.72	0.88
1:A:18:GLN:NE2	1:A:18:GLN:H	1.70	0.88
1:B:145:ARG:HG2	1:B:145:ARG:NH1	1.86	0.86
1:C:201:ILE:HG22	1:C:203:ALA:H	1.41	0.86
1:D:143:HIS:ND1	1:D:148:ASN:HB2	1.91	0.85
1:C:145:ARG:HG2	1:C:145:ARG:HH11	1.38	0.85
1:B:143:HIS:HD2	1:B:144:TYR:CD2	1.94	0.84
1:C:153:SER:OG	1:C:216:ASN:HB3	1.76	0.84
1:C:18:GLN:N	1:C:18:GLN:HE21	1.76	0.84
1:C:18:GLN:NE2	1:C:18:GLN:H	1.76	0.84
1:D:148:ASN:N	1:D:148:ASN:HD22	1.76	0.83
1:B:145:ARG:HH11	1:B:145:ARG:CG	1.91	0.83
1:A:130:MET:HE2	1:A:132:LEU:CD1	1.98	0.82
1:D:148:ASN:H	1:D:148:ASN:HD22	1.28	0.82
1:C:154:GLN:NE2	1:C:154:GLN:HA	1.96	0.80
1:C:145:ARG:HH11	1:C:145:ARG:CG	1.94	0.80
1:C:159:LEU:HD12	1:C:164:GLN:HG3	1.62	0.80
1:A:18:GLN:HE21	1:A:18:GLN:N	1.80	0.79
1:B:175:SER:HB3	1:B:178:GLU:HG3	1.64	0.79
1:C:199:LYS:H	1:C:199:LYS:HD3	1.47	0.79
1:D:127:GLN:O	1:D:128:ASP:HB2	1.85	0.77
1:D:100:PHE:CE2	1:D:143:HIS:HD2	2.04	0.76
1:C:133:THR:HG23	1:C:136:LEU:H	1.51	0.75
1:B:150:VAL:HG11	1:B:218:GLY:H	1.52	0.73
1:B:162:ARG:HH11	1:B:162:ARG:HG3	1.52	0.73
1:D:100:PHE:CD2	1:D:143:HIS:HD2	2.05	0.73
1:D:37:THR:HG21	1:D:45:GLU:HG3	1.71	0.73
1:C:161:LYS:HD2	1:C:161:LYS:N	2.04	0.72
1:C:198:PHE:O	1:C:202:ASN:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:VAL:HG12	1:B:201:ILE:HD12	1.71	0.72
1:A:156:TYR:OH	1:A:168:LYS:HE3	1.90	0.72
1:D:143:HIS:ND1	1:D:143:HIS:C	2.43	0.71
1:B:43:TRP:NE1	1:B:44:LEU:HD22	2.05	0.71
1:B:133:THR:CG2	1:B:136:LEU:H	2.02	0.71
1:D:207:LEU:HA	1:D:210:LEU:HD21	1.72	0.71
1:B:143:HIS:CD2	1:B:144:TYR:CD2	2.79	0.71
1:D:8:ASN:HB3	1:D:55:GLN:HG3	1.71	0.70
1:D:143:HIS:CE1	1:D:148:ASN:CB	2.73	0.70
1:C:148:ASN:N	1:C:148:ASN:HD22	1.88	0.70
1:B:201:ILE:O	1:B:202:ASN:CB	2.39	0.70
1:D:124:LYS:O	1:D:129:GLU:HG3	1.91	0.70
1:A:133:THR:CG2	1:A:136:LEU:H	2.04	0.70
1:C:186:SER:HB3	1:C:189:THR:OG1	1.91	0.70
1:B:133:THR:HG22	1:B:136:LEU:H	1.57	0.69
1:B:132:LEU:HD23	1:B:136:LEU:HD23	1.75	0.69
1:A:96:HIS:HB3	1:A:136:LEU:CD1	2.22	0.69
1:D:141:ILE:O	1:D:145:ARG:HB3	1.93	0.69
1:D:133:THR:HG22	1:D:135:LYS:N	2.08	0.68
1:C:199:LYS:N	1:C:199:LYS:HD3	2.09	0.68
1:B:43:TRP:CE2	1:B:44:LEU:HD22	2.30	0.67
1:B:177:ILE:HD12	1:B:177:ILE:H	1.59	0.66
1:C:148:ASN:ND2	1:C:148:ASN:N	2.44	0.66
1:A:127:GLN:HE22	1:C:6:LYS:HE3	1.60	0.65
1:A:133:THR:HG22	1:A:136:LEU:H	1.60	0.65
1:B:18:GLN:HE21	1:B:18:GLN:H	0.80	0.65
1:D:143:HIS:C	1:D:143:HIS:HD1	1.98	0.65
1:A:43:TRP:CE2	1:A:44:LEU:HG	2.32	0.65
1:A:13:SER:O	1:A:38:PRO:HA	1.97	0.65
1:B:132:LEU:CD2	1:B:136:LEU:HD23	2.27	0.65
1:B:75:PHE:O	1:B:79:SER:OG	2.14	0.64
1:D:100:PHE:CE2	1:D:143:HIS:CD2	2.86	0.64
1:A:31:PRO:HD2	1:A:126:LEU:HD23	1.78	0.64
1:D:87:ILE:HG12	1:D:105:LEU:HD11	1.81	0.63
1:A:31:PRO:HD2	1:A:126:LEU:CD2	2.30	0.62
1:A:76:LYS:HE2	1:A:80:CYS:O	1.98	0.62
1:C:156:TYR:OH	1:C:168:LYS:HE2	1.98	0.62
1:A:198:PHE:O	1:A:199:LYS:HD2	1.99	0.62
1:B:148:ASN:OD1	1:B:148:ASN:N	2.30	0.62
1:C:130:MET:CE	1:C:132:LEU:HD11	2.29	0.62
1:C:74:SER:O	1:C:78:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HE3	1:A:200:LYS:HA	1.80	0.62
1:C:185:VAL:CG1	1:C:189:THR:HB	2.29	0.61
1:D:148:ASN:N	1:D:148:ASN:ND2	2.46	0.61
1:C:27:GLU:HG2	1:C:32:LEU:O	2.00	0.60
1:D:9:VAL:HG21	1:D:32:LEU:HD22	1.83	0.60
1:B:59:ILE:HD13	1:B:102:TRP:CZ3	2.36	0.60
1:A:156:TYR:CE2	1:A:164:GLN:HG2	2.37	0.60
1:D:76:LYS:HE2	1:D:85:GLU:OE2	2.01	0.60
1:B:213:ALA:O	1:B:217:ILE:HG22	2.00	0.60
1:D:143:HIS:HD1	1:D:148:ASN:HB2	1.67	0.60
1:B:185:VAL:HG12	1:B:189:THR:HB	1.82	0.60
1:B:175:SER:HB3	1:B:178:GLU:CG	2.31	0.59
1:D:133:THR:CG2	1:D:135:LYS:H	2.16	0.59
1:B:10:ARG:HB3	1:B:57:LEU:HD23	1.85	0.59
1:B:120:LYS:O	1:B:123:SER:OG	2.18	0.58
1:B:137:ALA:O	1:B:141:ILE:HG13	2.03	0.58
1:D:123:SER:O	1:D:127:GLN:HG2	2.03	0.58
1:C:145:ARG:HG2	1:C:145:ARG:NH1	2.14	0.58
1:A:176:ASN:OD1	1:A:206:ARG:NH1	2.36	0.58
1:A:191:LYS:HZ2	1:A:191:LYS:HB2	1.67	0.58
1:A:75:PHE:O	1:A:79:SER:OG	2.22	0.58
1:A:27:GLU:HG2	1:A:32:LEU:O	2.04	0.58
1:C:137:ALA:O	1:C:141:ILE:HG13	2.04	0.57
1:D:49:PRO:HA	1:D:52:ARG:NH1	2.19	0.57
1:B:13:SER:O	1:B:38:PRO:HA	2.05	0.57
1:C:137:ALA:HB1	1:D:137:ALA:HB1	1.86	0.57
1:A:141:ILE:O	1:A:145:ARG:HB2	2.04	0.57
1:D:130:MET:CE	1:D:132:LEU:HD11	2.34	0.57
1:B:143:HIS:CE1	1:B:148:ASN:HB2	2.40	0.57
1:D:210:LEU:HD23	1:D:210:LEU:H	1.69	0.57
1:A:185:VAL:HG12	1:A:189:THR:HB	1.86	0.57
1:B:171:GLY:HA3	1:B:213:ALA:HB1	1.85	0.57
1:B:197:VAL:CG1	1:B:201:ILE:HD12	2.35	0.56
1:B:39:PHE:HB3	1:B:68:VAL:HG11	1.86	0.56
1:A:97:LYS:HA	1:A:100:PHE:CE2	2.40	0.56
1:A:186:SER:HB3	1:A:189:THR:OG1	2.05	0.56
1:D:137:ALA:O	1:D:141:ILE:HG13	2.05	0.56
1:D:143:HIS:HE1	1:D:148:ASN:C	2.09	0.56
1:C:96:HIS:HB2	1:C:139:GLU:HG2	1.87	0.56
1:A:39:PHE:HB3	1:A:68:VAL:HG11	1.88	0.56
1:D:39:PHE:O	1:D:42:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:HIS:CD2	1:B:144:TYR:CE2	2.94	0.56
1:C:8:ASN:HB3	1:C:55:GLN:HG3	1.87	0.56
1:B:31:PRO:HD2	1:B:126:LEU:HD23	1.87	0.55
1:C:9:VAL:HG13	1:C:56:MET:HE2	1.88	0.55
1:D:10:ARG:HB3	1:D:57:LEU:HD23	1.89	0.55
1:A:156:TYR:CD2	1:A:156:TYR:C	2.80	0.55
1:D:12:LEU:HA	1:D:37:THR:O	2.06	0.55
1:D:41:GLU:O	1:D:41:GLU:HG2	2.07	0.55
1:A:96:HIS:HB3	1:A:136:LEU:HD12	1.89	0.55
1:A:160:THR:HG23	1:A:163:GLU:CD	2.28	0.55
1:B:156:TYR:CE1	1:B:217:ILE:HD11	2.41	0.54
1:B:97:LYS:HA	1:B:100:PHE:CE2	2.42	0.54
1:A:49:PRO:HA	1:A:52:ARG:NH2	2.21	0.54
1:D:133:THR:HG22	1:D:135:LYS:H	1.70	0.54
1:D:52:ARG:HA	1:D:79:SER:O	2.07	0.54
1:C:31:PRO:HD2	1:C:126:LEU:CD2	2.36	0.54
1:C:85:GLU:OE2	1:C:102:TRP:HB3	2.07	0.54
1:A:148:ASN:OD1	1:A:148:ASN:N	2.41	0.54
1:A:154:GLN:O	1:A:158:LYS:HG3	2.06	0.54
1:D:207:LEU:HA	1:D:210:LEU:CD2	2.36	0.54
1:D:4:GLU:HG3	1:D:5:ASN:H	1.72	0.54
1:C:207:LEU:HA	1:C:210:LEU:HD23	1.89	0.54
1:D:9:VAL:HG12	1:D:10:ARG:N	2.23	0.54
1:B:43:TRP:CE2	1:B:44:LEU:CD2	2.91	0.53
1:B:154:GLN:O	1:B:158:LYS:HG3	2.08	0.53
1:D:95:GLU:HB3	1:D:98:LEU:HG	1.89	0.53
1:D:43:TRP:CE2	1:D:44:LEU:HG	2.43	0.53
1:B:19:SER:HB3	1:B:36:ILE:HD13	1.91	0.53
1:D:100:PHE:CD2	1:D:143:HIS:CD2	2.93	0.53
1:A:8:ASN:HB3	1:A:55:GLN:HG3	1.91	0.52
1:A:19:SER:HB3	1:A:36:ILE:HD13	1.91	0.52
1:B:144:TYR:O	1:B:147:GLY:N	2.40	0.52
1:C:31:PRO:HD2	1:C:126:LEU:HD23	1.91	0.52
1:C:19:SER:HB3	1:C:36:ILE:HD13	1.92	0.52
1:C:196:ASN:N	1:C:196:ASN:ND2	2.57	0.52
1:D:109:PHE:CE1	1:D:118:LEU:HA	2.44	0.52
1:B:168:LYS:HG2	1:B:217:ILE:HG13	1.91	0.52
1:C:154:GLN:CA	1:C:154:GLN:NE2	2.70	0.52
1:B:29:LYS:O	1:B:30:LEU:HD23	2.11	0.51
1:A:10:ARG:HB3	1:A:57:LEU:HD23	1.91	0.51
1:B:177:ILE:N	1:B:177:ILE:HD12	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ILE:HD13	1:D:140:TYR:CD2	2.46	0.51
1:A:94:ILE:HD13	1:A:95:GLU:N	2.26	0.51
1:D:212:TRP:CZ2	1:D:216:ASN:ND2	2.68	0.51
1:C:52:ARG:HA	1:C:79:SER:O	2.10	0.51
1:D:132:LEU:HD22	1:D:136:LEU:HD23	1.92	0.51
1:C:156:TYR:CD2	1:C:156:TYR:C	2.84	0.51
1:A:132:LEU:HD22	1:A:136:LEU:HD23	1.93	0.51
1:A:170:LEU:HD21	1:A:206:ARG:NH2	2.27	0.50
1:B:150:VAL:CG1	1:B:218:GLY:H	2.20	0.50
1:C:154:GLN:CA	1:C:154:GLN:HE21	2.24	0.50
1:C:180:ALA:HB1	1:C:185:VAL:O	2.11	0.50
1:C:169:LEU:HD12	1:C:179:ILE:HG23	1.92	0.50
1:C:92:GLN:OE1	1:C:110:TYR:HB3	2.11	0.50
1:B:207:LEU:HD12	1:B:210:LEU:HD23	1.92	0.50
1:C:212:TRP:O	1:C:216:ASN:HB2	2.12	0.50
1:C:196:ASN:N	1:C:196:ASN:HD22	2.07	0.50
1:D:130:MET:HE1	1:D:132:LEU:HD11	1.92	0.50
1:C:153:SER:HG	1:C:216:ASN:HB3	1.75	0.49
1:D:13:SER:O	1:D:38:PRO:HA	2.11	0.49
1:C:200:LYS:O	1:C:201:ILE:C	2.50	0.49
1:A:15:VAL:O	1:A:16:CYS:HB3	2.12	0.49
1:D:30:LEU:HD13	1:D:122:MET:HB3	1.95	0.49
1:A:11:MET:HB2	1:A:34:LEU:HD21	1.93	0.49
1:B:162:ARG:HG3	1:B:162:ARG:NH1	2.25	0.49
1:B:17:MET:CA	1:B:17:MET:HE3	2.43	0.49
1:C:165:GLN:O	1:C:169:LEU:HG	2.13	0.49
1:D:85:GLU:OE1	1:D:102:TRP:HE3	1.96	0.49
1:B:9:VAL:HG12	1:B:10:ARG:N	2.27	0.49
1:C:164:GLN:O	1:C:168:LYS:HG3	2.13	0.49
1:A:177:ILE:H	1:A:177:ILE:HD12	1.77	0.48
1:A:199:LYS:HA	1:A:199:LYS:HE3	1.95	0.48
1:B:202:ASN:OD1	1:B:202:ASN:O	2.30	0.48
1:C:145:ARG:CB	1:C:145:ARG:HH11	2.26	0.48
1:D:148:ASN:H	1:D:148:ASN:ND2	2.04	0.48
1:A:185:VAL:CG1	1:A:189:THR:HB	2.43	0.48
1:A:74:SER:O	1:A:78:ILE:HG12	2.14	0.48
1:C:154:GLN:HE21	1:C:154:GLN:HA	1.71	0.48
1:B:130:MET:HE2	1:B:132:LEU:HD11	1.88	0.48
1:D:206:ARG:O	1:D:210:LEU:HD23	2.14	0.48
1:C:41:GLU:HG3	1:C:44:LEU:HD12	1.96	0.47
1:C:49:PRO:HA	1:C:52:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PRO:HD2	1:B:126:LEU:CD2	2.44	0.47
1:A:185:VAL:HG12	1:A:186:SER:N	2.28	0.47
1:C:175:SER:HB3	1:C:178:GLU:HG3	1.97	0.47
1:D:132:LEU:HD22	1:D:136:LEU:CD2	2.44	0.47
1:A:44:LEU:O	1:A:48:LYS:HE3	2.15	0.47
1:B:17:MET:HB3	1:B:17:MET:HE2	1.77	0.47
1:B:17:MET:HA	1:B:17:MET:HE3	1.96	0.47
1:C:185:VAL:HG12	1:C:189:THR:HB	1.97	0.47
1:C:134:ARG:NH2	1:D:124:LYS:HD3	2.29	0.47
1:D:133:THR:CG2	1:D:134:ARG:N	2.77	0.47
1:D:49:PRO:HA	1:D:52:ARG:HH12	1.79	0.47
1:D:66:ASP:HA	1:D:69:LEU:HD12	1.97	0.47
1:B:185:VAL:HG12	1:B:186:SER:N	2.30	0.47
1:C:130:MET:HE1	1:C:132:LEU:HD11	1.96	0.46
1:D:143:HIS:HE1	1:D:148:ASN:CB	2.26	0.46
1:D:17:MET:HA	1:D:17:MET:HE3	1.96	0.46
1:A:132:LEU:CD2	1:A:136:LEU:HD23	2.46	0.46
1:C:74:SER:HB3	1:C:208:GLN:HG2	1.98	0.46
1:A:137:ALA:HB1	1:B:137:ALA:HB1	1.96	0.46
1:B:133:THR:HG23	1:B:135:LYS:N	2.31	0.46
1:B:165:GLN:O	1:B:169:LEU:HG	2.16	0.46
1:B:23:LYS:HE3	1:B:34:LEU:O	2.16	0.46
1:A:97:LYS:HA	1:A:100:PHE:CD2	2.51	0.46
1:A:16:CYS:O	1:A:17:MET:C	2.54	0.46
1:B:207:LEU:O	1:B:211:ILE:HG13	2.15	0.46
1:B:70:THR:HG21	1:B:201:ILE:O	2.16	0.46
1:C:138:GLN:OE1	1:D:129:GLU:HA	2.16	0.45
1:C:155:MET:HA	1:C:158:LYS:HG3	1.97	0.45
1:A:167:ILE:HA	1:A:167:ILE:HD12	1.85	0.45
1:A:198:PHE:O	1:A:202:ASN:N	2.48	0.45
1:C:199:LYS:CD	1:C:199:LYS:N	2.72	0.45
1:D:65:SER:OG	1:D:68:VAL:HG22	2.16	0.45
1:D:121:GLY:O	1:D:125:ILE:HG13	2.16	0.45
1:B:150:VAL:HG13	1:B:151:VAL:N	2.31	0.45
1:B:202:ASN:CG	1:B:202:ASN:O	2.55	0.45
1:D:87:ILE:HG12	1:D:105:LEU:CD1	2.46	0.45
1:B:124:LYS:O	1:B:127:GLN:HB2	2.16	0.45
1:B:180:ALA:HB1	1:B:185:VAL:O	2.17	0.45
1:A:18:GLN:NE2	1:A:18:GLN:N	2.50	0.45
1:B:177:ILE:HG13	1:B:187:GLU:HG3	1.98	0.45
1:A:49:PRO:HA	1:A:52:ARG:HH22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:HG22	1:D:136:LEU:H	1.81	0.45
1:D:143:HIS:HE1	1:D:148:ASN:HB2	1.67	0.45
1:D:212:TRP:O	1:D:216:ASN:HB2	2.17	0.45
1:D:61:TYR:O	1:D:64:ILE:HG22	2.16	0.45
1:C:133:THR:HG22	1:C:136:LEU:HB3	1.98	0.44
1:B:156:TYR:CE1	1:B:217:ILE:CD1	3.00	0.44
1:D:43:TRP:CH2	1:D:44:LEU:HD21	2.52	0.44
1:B:162:ARG:CG	1:B:162:ARG:NH1	2.78	0.44
1:C:13:SER:O	1:C:38:PRO:HA	2.18	0.44
1:B:161:LYS:HD2	1:B:161:LYS:H	1.82	0.44
1:B:11:MET:HB2	1:B:34:LEU:HD21	1.98	0.44
1:B:161:LYS:HD2	1:B:161:LYS:N	2.32	0.44
1:B:156:TYR:CZ	1:B:217:ILE:HD11	2.52	0.44
1:B:212:TRP:CD1	1:B:216:ASN:ND2	2.86	0.44
1:A:156:TYR:CZ	1:A:164:GLN:HG2	2.52	0.43
1:C:52:ARG:HG3	1:C:52:ARG:HH21	1.84	0.43
1:D:30:LEU:HA	1:D:31:PRO:HD3	1.82	0.43
1:A:133:THR:HG23	1:A:135:LYS:N	2.33	0.43
1:A:50:GLU:CD	1:A:50:GLU:H	2.22	0.43
1:C:41:GLU:O	1:C:41:GLU:HG2	2.19	0.43
1:D:199:LYS:HA	1:D:200:LYS:HA	1.73	0.43
1:A:122:MET:HE2	1:A:122:MET:HB3	1.41	0.43
1:B:209:ALA:O	1:B:212:TRP:HB3	2.19	0.43
1:C:23:LYS:CE	1:C:34:LEU:O	2.66	0.43
1:D:50:GLU:H	1:D:50:GLU:CD	2.22	0.43
1:B:70:THR:HG21	1:B:202:ASN:HB3	2.00	0.43
1:C:145:ARG:HH11	1:C:145:ARG:HB3	1.83	0.43
1:B:97:LYS:HA	1:B:100:PHE:CD2	2.52	0.43
1:B:156:TYR:CD1	1:B:217:ILE:CD1	3.01	0.43
1:B:167:ILE:HD12	1:B:167:ILE:HA	1.92	0.43
1:B:8:ASN:OD1	1:B:54:ILE:HA	2.18	0.43
1:C:215:ASN:O	1:C:216:ASN:OD1	2.36	0.43
1:D:34:LEU:HD23	1:D:35:GLU:N	2.34	0.43
1:B:150:VAL:CG1	1:B:151:VAL:N	2.82	0.43
1:C:48:LYS:HA	1:C:49:PRO:HD3	1.86	0.43
1:D:11:MET:HB2	1:D:34:LEU:HD21	2.00	0.43
1:C:142:LEU:HD12	1:C:142:LEU:HA	1.72	0.42
1:B:162:ARG:HA	1:B:162:ARG:HD3	1.83	0.42
1:B:43:TRP:CH2	1:B:44:LEU:HD11	2.55	0.42
1:C:9:VAL:HG21	1:C:32:LEU:HD22	2.01	0.42
1:A:119:ILE:HD13	1:A:119:ILE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HA	1:A:199:LYS:CE	2.49	0.42
1:B:198:PHE:CD1	1:B:198:PHE:N	2.86	0.42
1:C:159:LEU:CD1	1:C:164:GLN:HG3	2.42	0.42
1:A:156:TYR:HD2	1:A:157:ALA:N	2.16	0.42
1:B:92:GLN:NE2	1:B:112:ASP:OD1	2.47	0.42
1:B:180:ALA:HB2	1:B:187:GLU:HA	2.00	0.42
1:C:176:ASN:OD1	1:C:206:ARG:NH1	2.52	0.42
1:B:30:LEU:HA	1:B:31:PRO:HD3	1.86	0.42
1:A:200:LYS:C	1:A:202:ASN:N	2.73	0.42
1:D:17:MET:HE3	1:D:17:MET:CA	2.49	0.42
1:D:115:MET:O	1:D:119:ILE:HG12	2.20	0.42
1:A:104:ASN:O	1:A:105:LEU:C	2.58	0.42
1:A:160:THR:HG23	1:A:163:GLU:OE1	2.20	0.42
1:A:87:ILE:HD13	1:A:105:LEU:HD13	2.02	0.42
1:B:120:LYS:O	1:B:124:LYS:HG3	2.20	0.42
1:D:210:LEU:O	1:D:213:ALA:HB3	2.20	0.42
1:B:177:ILE:H	1:B:177:ILE:CD1	2.31	0.41
1:A:156:TYR:CE1	1:A:217:ILE:HD13	2.55	0.41
1:A:48:LYS:HA	1:A:49:PRO:HD3	1.83	0.41
1:A:61:TYR:O	1:A:64:ILE:HG22	2.20	0.41
1:B:212:TRP:NE1	1:B:216:ASN:ND2	2.69	0.41
1:A:120:LYS:O	1:A:123:SER:OG	2.31	0.41
1:C:44:LEU:O	1:C:48:LYS:HE3	2.20	0.41
1:D:52:ARG:HG2	1:D:79:SER:O	2.20	0.41
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.82	0.41
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.85	0.41
1:A:127:GLN:NE2	1:C:6:LYS:HE3	2.32	0.41
1:A:197:VAL:C	1:A:199:LYS:N	2.74	0.41
1:B:218:GLY:HA2	1:B:219:ILE:HA	1.84	0.41
1:C:161:LYS:HD2	1:C:161:LYS:H	1.81	0.41
1:A:43:TRP:CH2	1:A:44:LEU:HD21	2.56	0.41
1:A:85:GLU:OE2	1:A:102:TRP:HB3	2.20	0.41
1:D:37:THR:HA	1:D:38:PRO:HD3	1.91	0.41
1:B:145:ARG:CG	1:B:145:ARG:NH1	2.62	0.41
1:B:66:ASP:HB3	1:B:155:MET:CE	2.50	0.41
1:B:111:ILE:HG22	1:B:112:ASP:N	2.36	0.41
1:B:144:TYR:N	1:B:144:TYR:CD2	2.89	0.41
1:B:9:VAL:HG13	1:B:56:MET:HB3	2.03	0.41
1:A:65:SER:O	1:A:68:VAL:HG22	2.21	0.41
1:A:159:LEU:HB3	1:A:163:GLU:HB2	2.03	0.40
1:B:7:LEU:HA	1:B:7:LEU:HD12	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LEU:HD12	1:C:7:LEU:HA	1.94	0.40
1:C:122:MET:HB3	1:C:122:MET:HE3	1.83	0.40
1:B:43:TRP:CZ2	1:B:44:LEU:HD21	2.57	0.40
1:C:21:LEU:HA	1:C:21:LEU:HD12	1.71	0.40
1:B:6:LYS:HB3	1:B:6:LYS:HE3	1.87	0.40
1:C:153:SER:OG	1:C:216:ASN:CB	2.60	0.40
1:C:185:VAL:HG12	1:C:186:SER:O	2.21	0.40
1:D:138:GLN:O	1:D:142:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/225 (96%)	203 (94%)	12 (6%)	0	100	100
1	B	213/225 (95%)	198 (93%)	14 (7%)	1 (0%)	29	61
1	C	211/225 (94%)	200 (95%)	9 (4%)	2 (1%)	17	49
1	D	169/225 (75%)	152 (90%)	17 (10%)	0	100	100
All	All	808/900 (90%)	753 (93%)	52 (6%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	ASN
1	C	143	HIS
1	C	201	ILE



### 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	199/207 (96%)	170 (85%)	29 (15%)	3	13
1	B	197/207 (95%)	168 (85%)	29 (15%)	3	12
1	C	196/207 (95%)	161 (82%)	35 (18%)	2	7
1	D	161/207 (78%)	144 (89%)	17 (11%)	6	24
All	All	753/828 (91%)	643 (85%)	110 (15%)	3	13

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	10	ARG
1	A	15	VAL
1	A	17	MET
1	A	18	GLN
1	A	19	SER
1	A	29	LYS
1	A	42	LEU
1	A	50	GLU
1	A	55	GLN
1	A	67	ASP
1	A	76	LYS
1	A	79	SER
1	A	85	GLU
1	A	94	ILE
1	A	101	LYS
1	A	116	ASP
1	A	132	LEU
1	A	133	THR
1	A	148	ASN
1	A	151	VAL
1	A	160	THR
1	A	161	LYS
1	A	162	ARG

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Mol	Chain	Res	Type
1	A	170	LEU
1	A	186	SER
1	A	190	VAL
1	A	202	ASN
1	A	219	ILE
1	B	5	ASN
1	B	6	LYS
1	B	10	ARG
1	B	15	VAL
1	B	18	GLN
1	B	29	LYS
1	B	32	LEU
1	B	35	GLU
1	B	44	LEU
1	B	67	ASP
1	B	70	THR
1	B	73	SER
1	B	79	SER
1	B	111	ILE
1	B	126	LEU
1	B	133	THR
1	B	134	ARG
1	B	142	LEU
1	B	145	ARG
1	B	148	ASN
1	B	150	VAL
1	B	151	VAL
1	B	159	LEU
1	B	161	LYS
1	B	162	ARG
1	B	170	LEU
1	B	190	VAL
1	B	210	LEU
1	B	217	ILE
1	C	4	GLU
1	C	10	ARG
1	C	17	MET
1	C	18	GLN
1	C	19	SER
1	C	23	LYS
1	C	28	SER
1	C	29	LYS

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Mol	Chain	Res	Type
1	C	35	GLU
1	C	55	GLN
1	C	66	ASP
1	C	70	THR
1	C	76	LYS
1	C	87	ILE
1	C	94	ILE
1	C	101	LYS
1	C	111	ILE
1	C	130	MET
1	C	139	GLU
1	C	142	LEU
1	C	145	ARG
1	C	148	ASN
1	C	152	THR
1	C	153	SER
1	C	154	GLN
1	C	159	LEU
1	C	161	LYS
1	C	162	ARG
1	C	170	LEU
1	C	190	VAL
1	C	199	LYS
1	C	200	LYS
1	C	201	ILE
1	C	202	ASN
1	C	210	LEU
1	D	5	ASN
1	D	10	ARG
1	D	17	MET
1	D	18	GLN
1	D	35	GLU
1	D	50	GLU
1	D	71	ASP
1	D	92	GLN
1	D	123	SER
1	D	129	GLU
1	D	133	THR
1	D	143	HIS
1	D	145	ARG
1	D	148	ASN
1	D	151	VAL

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Mol	Chain	Res	Type
1	D	197	VAL
1	D	199	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	18	GLN
1	A	77	HIS
1	A	92	GLN
1	A	127	GLN
1	A	154	GLN
1	B	5	ASN
1	B	18	GLN
1	B	103	ASN
1	B	104	ASN
1	B	143	HIS
1	C	18	GLN
1	C	55	GLN
1	C	89	ASN
1	C	103	ASN
1	C	148	ASN
1	C	154	GLN
1	C	196	ASN
1	D	5	ASN
1	D	8	ASN
1	D	18	GLN
1	D	103	ASN
1	D	143	HIS
1	D	148	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 [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, 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	217/225 (96%)	0.08	1 (0%) 91 80	33, 58, 93, 126	0
1	B	215/225 (95%)	0.16	3 (1%) 75 55	39, 62, 109, 121	0
1	C	213/225 (94%)	0.43	13 (6%) 21 9	47, 80, 121, 135	0
1	D	173/225 (76%)	0.81	27 (15%) 2 1	60, 84, 125, 137	0
All	All	818/900 (90%)	0.35	44 (5%) 25 11	33, 74, 118, 137	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	GLY	6.9
1	A	3	ASP	6.7
1	D	151	VAL	5.7
1	D	210	LEU	5.5
1	D	148	ASN	4.5
1	C	149	SER	4.3
1	D	215	ASN	4.3
1	C	150	VAL	4.2
1	D	208	GLN	4.2
1	D	147	GLY	4.1
1	D	201	ILE	4.0
1	D	203	ALA	3.7
1	D	150	VAL	3.7
1	D	213	ALA	3.5
1	B	217	ILE	3.5
1	C	215	ASN	3.5
1	D	209	ALA	3.5
1	D	204	LYS	3.4
1	D	152	THR	3.3
1	D	197	VAL	3.3
1	D	207	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	8	ASN	3.1
1	D	195	HIS	3.1
1	D	211	ILE	3.0
1	D	202	ASN	2.8
1	D	196	ASN	2.8
1	C	214	LYS	2.7
1	C	201	ILE	2.5
1	C	166	ILE	2.5
1	C	159	LEU	2.5
1	C	148	ASN	2.4
1	C	184	PHE	2.4
1	D	82	ASP	2.3
1	C	158	LYS	2.3
1	D	212	TRP	2.3
1	B	218	GLY	2.3
1	C	197	VAL	2.3
1	D	194	LEU	2.2
1	C	200	LYS	2.2
1	B	159	LEU	2.1
1	D	200	LYS	2.1
1	D	214	LYS	2.0
1	D	205	ASN	2.0
1	D	149	SER	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.