



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 03:41 PM EDT

PDB ID : 6DKT  
Title : Crystal structure of Arginase from Bacillus subtilis  
Authors : Lewis, M.C.; Hollingsworth, S.A.; Holden, J.K.; Poulos, T.L.  
Deposited on : 2018-05-30  
Resolution : 2.08 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.

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  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

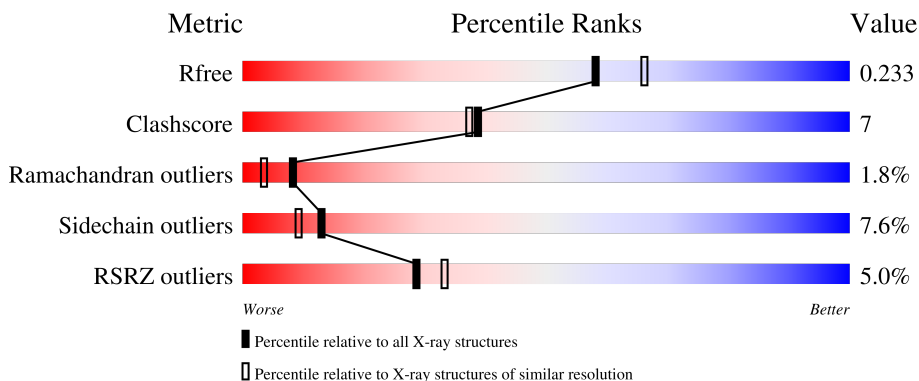
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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.



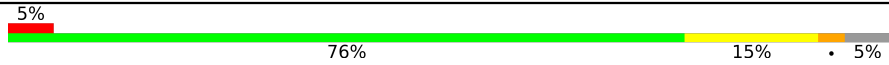
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 of 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	296	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6%      73%      19%      . .</p>
1	B	296	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5%      75%      17%      . .</p>
1	C	296	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      81%      12%      . .</p>
1	D	296	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3%      74%      19%      . .</p>
1	E	296	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      74%      12%      . 9%</p>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	296	 A horizontal bar chart showing the quality of chain. The bar is divided into segments: a small red segment at the beginning labeled '5%', a large green segment labeled '76%', a yellow segment labeled '15%', and a small grey segment at the end labeled '5%'.

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 25345 atoms, of which 12220 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 Arginase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	283	4174	1335	2056	356	416	11	0	0	0
1	B	283	4173	1336	2052	358	416	11	0	0	0
1	C	283	4153	1329	2046	354	413	11	0	0	0
1	D	283	4180	1336	2060	357	416	11	0	0	0
1	E	268	3982	1271	1971	335	394	11	0	0	0
1	F	280	4136	1325	2035	354	411	11	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

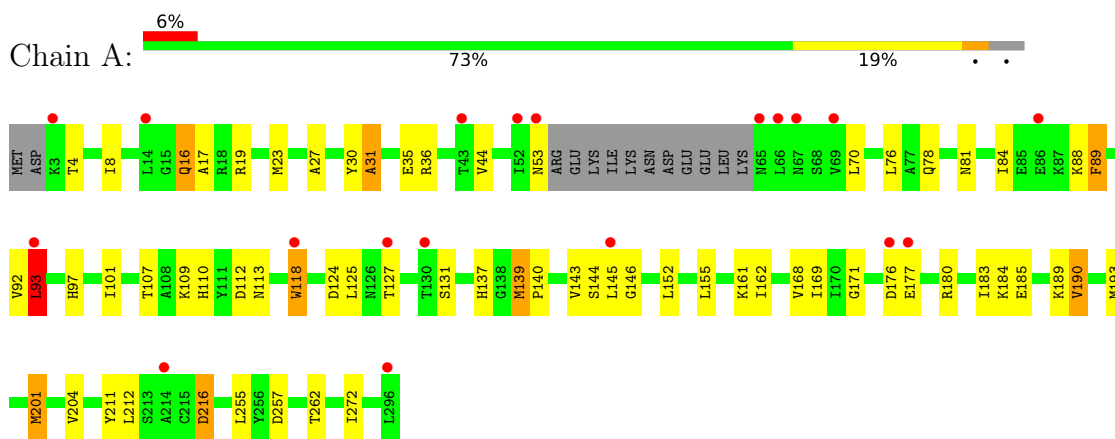
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	71	Total O 71 71	0	0
3	B	102	Total O 102 102	0	0
3	C	77	Total O 77 77	0	0
3	D	110	Total O 110 110	0	0
3	E	86	Total O 86 86	0	0
3	F	89	Total O 89 89	0	0

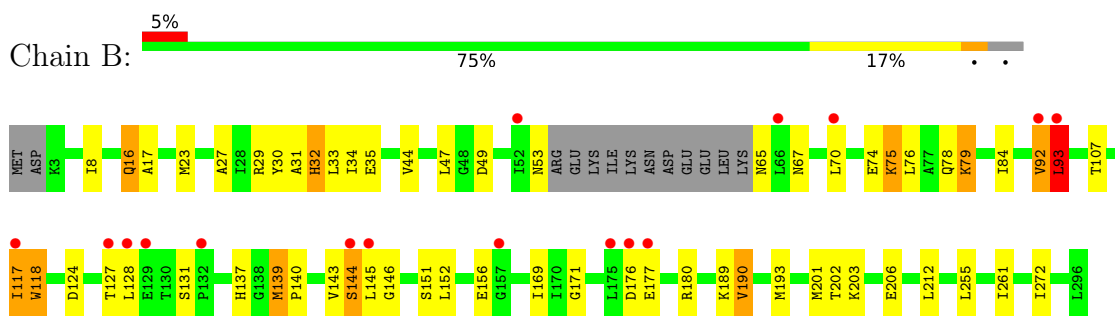
### 3 Residue-property plots [i](#)

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.

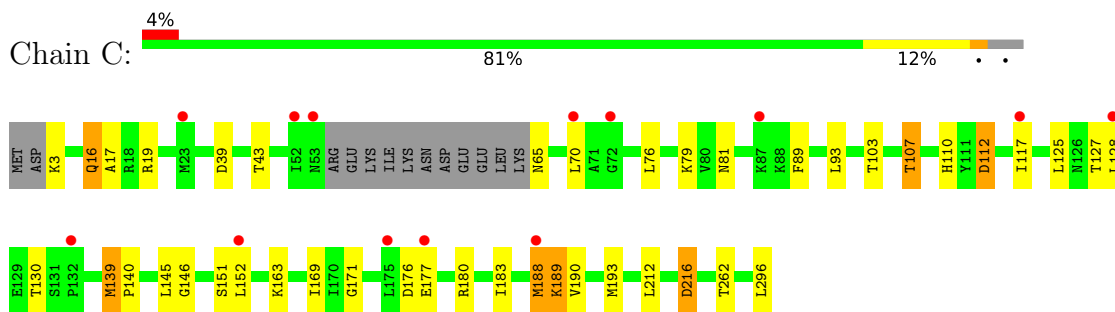
- Molecule 1: Arginase



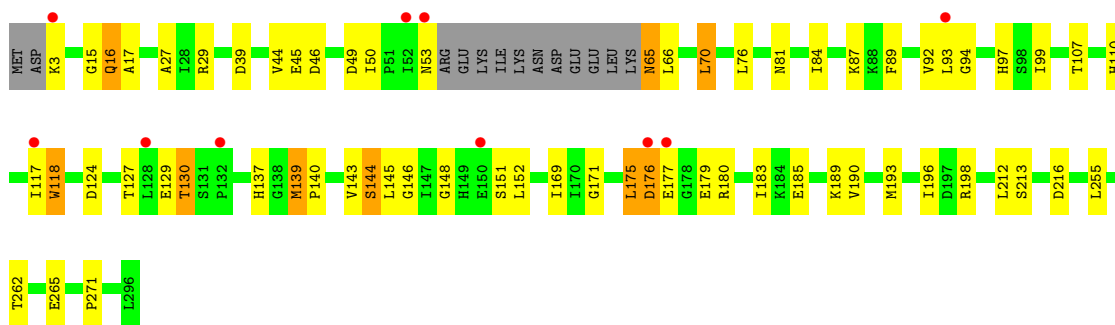
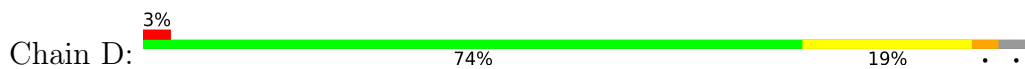
- Molecule 1: Arginase



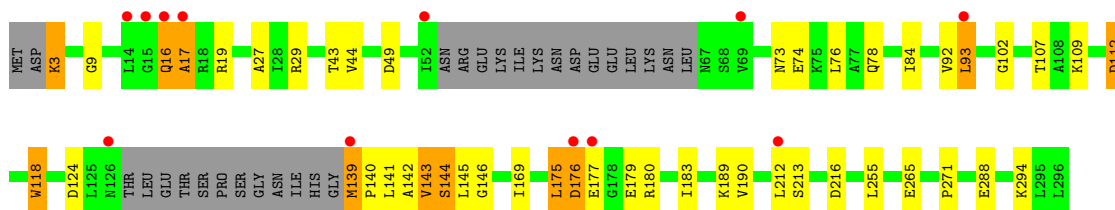
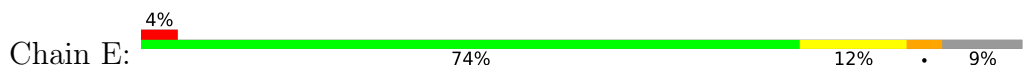
- Molecule 1: Arginase



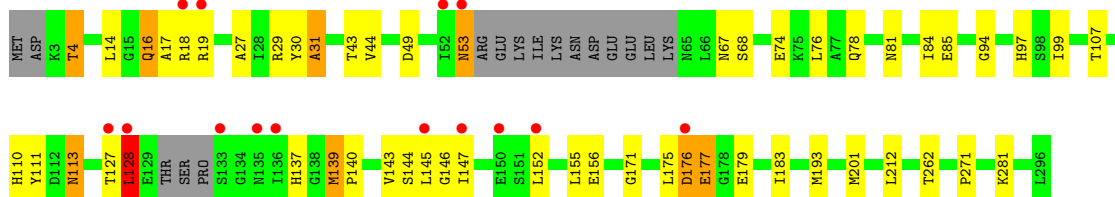
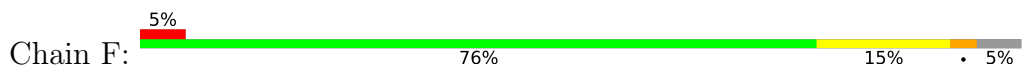
- Molecule 1: Arginase



- Molecule 1: Arginase



- Molecule 1: Arginase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.14Å 128.55Å 82.02Å 90.00° 112.69° 90.00°	Depositor
Resolution (Å)	47.70 – 2.08 48.99 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.70-2.08) 94.9 (48.99-2.08)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.08Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.204 , 0.231 0.205 , 0.233	Depositor DCC
$R_{free}$ test set	2009 reflections (2.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtrriage
Anisotropy	0.394	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25345	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.26	0/2152	0.51	1/2917 (0.0%)
1	B	0.26	0/2155	0.51	0/2919
1	C	0.25	0/2141	0.49	0/2903
1	D	0.27	0/2154	0.49	0/2918
1	E	0.27	0/2042	0.50	0/2765
1	F	0.26	0/2133	0.48	0/2887
All	All	0.26	0/12777	0.50	1/17309 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	LEU	CA-CB-CG	5.21	127.29	115.30

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	2118	2056	2104	37	0
1	B	2121	2052	2113	39	1
1	C	2107	2046	2082	22	0
1	D	2120	2060	2108	35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2011	1971	1997	28	1
1	F	2101	2035	2093	31	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	71	0	0	5	1
3	B	102	0	0	9	0
3	C	77	0	0	6	0
3	D	110	0	0	8	2
3	E	86	0	0	5	1
3	F	89	0	0	6	0
All	All	13125	12220	12497	187	3

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 7.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ASP:O	3:D:601:HOH:O	1.85	0.93
1:B:201:MET:SD	3:B:684:HOH:O	2.30	0.90
1:F:143:VAL:O	1:F:144:SER:OG	1.91	0.89
1:E:78:GLN:OE1	3:E:601:HOH:O	1.93	0.86
1:F:85:GLU:OE1	3:F:601:HOH:O	1.97	0.82
1:F:176:ASP:O	3:F:602:HOH:O	1.99	0.80
1:F:78:GLN:NE2	1:F:156:GLU:OE2	2.15	0.79
1:A:176:ASP:O	3:A:601:HOH:O	2.03	0.76
1:C:39:ASP:OD2	3:C:601:HOH:O	2.03	0.76
1:D:3:LYS:N	3:D:604:HOH:O	2.18	0.76
1:C:3:LYS:NZ	3:C:605:HOH:O	2.19	0.74
1:C:262:THR:OG1	3:C:602:HOH:O	2.05	0.74
1:A:113:ASN:N	1:A:216:ASP:OD2	2.23	0.72
1:E:3:LYS:O	3:E:602:HOH:O	2.10	0.69
1:D:65:ASN:N	3:D:606:HOH:O	2.26	0.68
1:B:67:ASN:OD1	3:B:602:HOH:O	2.11	0.67
1:C:176:ASP:O	3:C:603:HOH:O	2.12	0.67
1:F:145:LEU:N	1:F:146:GLY:HA2	2.10	0.66
1:B:78:GLN:NE2	1:B:156:GLU:OE2	2.28	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASN:OD1	3:C:604:HOH:O	2.13	0.66
1:A:145:LEU:N	1:A:146:GLY:HA2	2.12	0.65
1:B:145:LEU:N	1:B:146:GLY:HA2	2.11	0.65
1:C:145:LEU:N	1:C:146:GLY:HA2	2.12	0.64
1:B:32:HIS:O	1:B:34:ILE:N	2.31	0.63
1:D:87:LYS:O	3:D:603:HOH:O	2.14	0.63
1:A:211:TYR:OH	3:A:602:HOH:O	2.16	0.62
1:F:113:ASN:ND2	3:F:604:HOH:O	2.15	0.62
1:D:145:LEU:N	1:D:146:GLY:HA2	2.15	0.62
1:B:84:ILE:HD11	1:B:107:THR:HG22	1.82	0.61
1:D:84:ILE:HD11	1:D:107:THR:HG22	1.82	0.61
1:D:3:LYS:N	3:D:608:HOH:O	2.32	0.61
1:E:145:LEU:N	1:E:146:GLY:HA2	2.16	0.60
1:F:281:LYS:NZ	3:F:603:HOH:O	2.13	0.59
1:B:143:VAL:O	1:B:144:SER:CB	2.50	0.59
1:F:84:ILE:HD11	1:F:107:THR:HG22	1.85	0.59
1:B:206:GLU:OE1	3:B:604:HOH:O	2.17	0.58
1:F:171:GLY:HA2	1:F:193:MET:CE	2.33	0.58
1:B:171:GLY:HA2	1:B:193:MET:CE	2.35	0.57
1:E:139:MET:N	3:E:605:HOH:O	2.37	0.56
1:E:288:GLU:OE1	3:E:603:HOH:O	2.18	0.56
1:F:144:SER:HB3	3:F:641:HOH:O	2.06	0.55
1:C:127:THR:H	1:C:130:THR:HG22	1.73	0.54
1:B:67:ASN:ND2	3:B:610:HOH:O	2.40	0.54
1:D:180:ARG:NH1	1:E:294:LYS:O	2.39	0.54
1:E:118:TRP:CH2	1:E:124:ASP:HB2	2.42	0.54
1:A:171:GLY:HA2	1:A:193:MET:CE	2.36	0.54
1:A:84:ILE:HD11	1:A:107:THR:HG22	1.89	0.53
1:E:139:MET:N	1:E:140:PRO:CD	2.71	0.53
1:F:94:GLY:HA3	1:F:99:ILE:HD13	1.90	0.53
1:C:139:MET:N	1:C:140:PRO:CD	2.72	0.53
1:B:139:MET:N	1:B:140:PRO:CD	2.72	0.52
1:D:143:VAL:O	1:D:144:SER:CB	2.56	0.52
1:B:27:ALA:O	1:B:30:TYR:O	2.27	0.52
1:E:139:MET:N	3:E:607:HOH:O	2.41	0.52
1:F:30:TYR:O	1:F:31:ALA:CB	2.57	0.52
1:D:171:GLY:HA2	1:D:193:MET:CE	2.40	0.52
1:F:139:MET:N	1:F:140:PRO:CD	2.72	0.52
1:D:139:MET:N	1:D:140:PRO:CD	2.73	0.52
1:A:30:TYR:O	1:A:31:ALA:CB	2.58	0.51
1:A:143:VAL:O	1:A:144:SER:CB	2.58	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:MET:HE2	1:A:204:VAL:HB	1.93	0.51
1:B:118:TRP:CH2	1:B:124:ASP:HB2	2.45	0.51
1:B:203:LYS:NZ	3:B:605:HOH:O	2.26	0.51
1:E:84:ILE:HD11	1:E:107:THR:HG22	1.92	0.51
1:F:81:ASN:OD1	1:F:110:HIS:NE2	2.42	0.51
1:B:131:SER:OG	3:B:603:HOH:O	2.12	0.50
1:A:139:MET:N	1:A:140:PRO:CD	2.74	0.50
1:A:88:LYS:O	1:A:89:PHE:HB3	2.12	0.50
1:C:81:ASN:OD1	1:C:110:HIS:NE2	2.40	0.50
1:E:9:GLY:HA2	1:E:93:LEU:HD23	1.94	0.50
1:E:143:VAL:O	1:E:144:SER:HB2	2.10	0.50
1:D:92:VAL:O	1:D:265:GLU:HA	2.11	0.50
1:A:35:GLU:OE1	1:A:36:ARG:NH1	2.44	0.50
1:E:176:ASP:HA	1:E:180:ARG:CD	2.41	0.50
1:C:171:GLY:HA2	1:C:193:MET:CE	2.42	0.49
1:D:46:ASP:OD2	3:D:605:HOH:O	2.19	0.49
1:D:143:VAL:O	1:D:144:SER:HB2	2.12	0.49
1:E:92:VAL:O	1:E:265:GLU:HA	2.12	0.49
1:E:29:ARG:NH1	1:E:49:ASP:OD2	2.43	0.49
1:B:140:PRO:O	1:B:143:VAL:O	2.30	0.49
1:E:175:LEU:O	1:E:176:ASP:O	2.31	0.49
1:D:140:PRO:O	1:D:143:VAL:O	2.31	0.48
1:A:145:LEU:HD23	1:A:162:ILE:HG13	1.95	0.48
1:A:88:LYS:O	1:A:89:PHE:CB	2.62	0.48
1:A:127:THR:O	1:A:131:SER:N	2.46	0.48
1:D:70:LEU:HD21	1:D:151:SER:HB2	1.96	0.48
1:C:188:MET:O	1:C:189:LYS:CB	2.61	0.48
1:E:179:GLU:O	1:E:183:ILE:HG12	2.14	0.48
1:F:84:ILE:HD12	1:F:107:THR:HA	1.95	0.48
1:F:143:VAL:C	1:F:144:SER:HG	2.06	0.48
1:A:30:TYR:O	1:A:31:ALA:HB3	2.15	0.47
1:A:93:LEU:C	1:A:93:LEU:HD23	2.35	0.47
1:F:74:GLU:HG3	1:F:155:LEU:HD11	1.97	0.47
1:B:16:GLN:HG2	1:B:17:ALA:N	2.30	0.47
1:B:93:LEU:HD23	1:B:93:LEU:O	2.15	0.47
1:B:176:ASP:HA	1:B:180:ARG:CD	2.44	0.47
1:A:8:ILE:O	1:A:92:VAL:O	2.33	0.47
1:B:74:GLU:HG3	3:B:634:HOH:O	2.15	0.47
1:A:101:ILE:HG22	1:A:155:LEU:HD22	1.97	0.46
1:A:184:LYS:HD3	1:F:111:TYR:CD1	2.50	0.46
1:D:81:ASN:OD1	1:D:110:HIS:NE2	2.42	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD21	1:B:151:SER:HB2	1.97	0.46
1:D:29:ARG:NH1	1:D:49:ASP:OD2	2.42	0.46
1:E:216:ASP:OD1	1:E:216:ASP:N	2.47	0.46
1:B:8:ILE:O	1:B:92:VAL:O	2.34	0.46
1:B:30:TYR:CD1	1:B:30:TYR:N	2.82	0.46
1:E:213:SER:CB	1:F:53:ASN:HB2	2.45	0.46
1:F:29:ARG:NH1	1:F:49:ASP:OD2	2.47	0.46
1:A:185:GLU:OE1	3:A:604:HOH:O	2.21	0.46
1:C:16:GLN:HG2	1:C:17:ALA:N	2.31	0.46
1:B:117:ILE:HD11	1:B:261:ILE:HD11	1.97	0.46
1:D:262:THR:OG1	3:D:602:HOH:O	2.08	0.46
1:A:27:ALA:O	1:A:30:TYR:O	2.34	0.45
1:A:125:LEU:CD1	1:A:183:ILE:HD11	2.46	0.45
1:B:30:TYR:O	1:B:31:ALA:HB3	2.16	0.45
1:D:94:GLY:HA3	1:D:99:ILE:HD13	1.99	0.45
1:F:4:THR:OG1	1:F:43:THR:OG1	2.35	0.45
1:B:118:TRP:HH2	1:B:124:ASP:OD2	1.99	0.45
1:C:169:ILE:HB	1:C:190:VAL:HB	1.99	0.45
1:A:16:GLN:HG2	1:A:17:ALA:N	2.31	0.45
1:F:27:ALA:O	1:F:30:TYR:O	2.34	0.45
1:D:15:GLY:HA2	3:D:634:HOH:O	2.17	0.45
1:A:155:LEU:O	1:A:161:LYS:NZ	2.46	0.44
1:D:127:THR:H	1:D:130:THR:HG22	1.82	0.44
1:D:169:ILE:HB	1:D:190:VAL:HB	1.99	0.44
1:B:202:THR:HB	3:B:667:HOH:O	2.18	0.44
1:D:118:TRP:CH2	1:D:124:ASP:HB2	2.53	0.44
1:D:216:ASP:OD1	1:D:216:ASP:N	2.47	0.44
1:A:23:MET:HE3	1:A:272:ILE:HG12	1.99	0.44
1:D:27:ALA:HB2	1:D:271:PRO:HG3	1.97	0.44
1:B:145:LEU:N	1:B:146:GLY:CA	2.79	0.44
1:B:32:HIS:HB3	1:B:35:GLU:HG2	1.99	0.44
1:B:169:ILE:HB	1:B:190:VAL:HB	1.98	0.44
1:E:27:ALA:HB2	1:E:271:PRO:HG3	2.00	0.44
1:F:30:TYR:CD1	1:F:30:TYR:N	2.85	0.43
1:E:16:GLN:HG2	1:E:17:ALA:N	2.34	0.43
1:F:145:LEU:N	1:F:146:GLY:CA	2.81	0.43
1:D:175:LEU:O	1:D:176:ASP:O	2.37	0.43
1:E:142:ALA:C	1:E:143:VAL:O	2.57	0.43
1:A:93:LEU:HD23	1:A:93:LEU:O	2.19	0.43
1:A:176:ASP:HA	1:A:180:ARG:CD	2.48	0.43
1:A:257:ASP:OD1	3:A:605:HOH:O	2.21	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:THR:O	1:C:107:THR:HG23	2.19	0.43
1:D:129:GLU:OE2	1:D:129:GLU:N	2.51	0.43
1:E:73:ASN:OD1	1:E:102:GLY:N	2.48	0.43
1:B:31:ALA:O	1:B:32:HIS:HB2	2.19	0.43
1:B:47:LEU:CB	1:B:79:LYS:HE2	2.49	0.43
1:A:81:ASN:OD1	1:A:110:HIS:NE2	2.49	0.42
1:B:180:ARG:HG2	1:C:296:LEU:HD12	2.01	0.42
1:B:23:MET:HE3	1:B:272:ILE:HG12	2.01	0.42
1:B:143:VAL:O	1:B:144:SER:HB3	2.17	0.42
1:F:14:LEU:HD13	1:F:68:SER:HB2	1.99	0.42
1:F:27:ALA:HB2	1:F:271:PRO:HG3	2.01	0.42
1:A:112:ASP:N	1:A:216:ASP:OD2	2.52	0.42
1:E:216:ASP:HA	1:F:67:ASN:ND2	2.33	0.42
1:A:118:TRP:CH2	1:A:124:ASP:HB2	2.54	0.42
1:D:193:MET:HE1	1:D:196:ILE:HD12	2.01	0.42
1:F:179:GLU:O	1:F:183:ILE:HG12	2.19	0.42
1:C:70:LEU:HD21	1:C:151:SER:HB2	2.01	0.42
1:D:84:ILE:HD12	1:D:107:THR:HA	2.00	0.42
1:F:127:THR:HG22	1:F:128:LEU:N	2.34	0.42
1:A:176:ASP:HA	1:A:180:ARG:HD3	2.02	0.42
1:B:124:ASP:HB3	1:B:140:PRO:HD2	2.01	0.41
1:E:169:ILE:HB	1:E:190:VAL:HB	2.02	0.41
1:B:127:THR:HG22	1:B:128:LEU:N	2.35	0.41
1:B:29:ARG:NH1	1:B:49:ASP:OD2	2.54	0.41
1:C:176:ASP:HA	1:C:180:ARG:HD3	2.02	0.41
1:D:16:GLN:HG2	1:D:17:ALA:N	2.35	0.41
1:E:93:LEU:HD23	1:E:93:LEU:O	2.21	0.41
1:E:141:LEU:O	1:E:143:VAL:O	2.37	0.41
1:C:216:ASP:OD1	1:C:216:ASP:N	2.35	0.41
1:A:168:VAL:HA	1:A:189:LYS:O	2.21	0.41
1:D:97:HIS:CE1	1:D:118:TRP:CH2	3.09	0.41
1:E:112:ASP:N	1:E:216:ASP:OD2	2.51	0.41
1:A:4:THR:O	1:A:88:LYS:O	2.38	0.40
1:C:112:ASP:N	1:C:216:ASP:OD2	2.51	0.40
1:D:179:GLU:O	1:D:183:ILE:HG12	2.21	0.40
1:C:125:LEU:CD1	1:C:183:ILE:HD11	2.51	0.40
1:C:176:ASP:N	3:C:603:HOH:O	2.54	0.40
1:F:262:THR:OG1	3:F:605:HOH:O	2.17	0.40
1:A:169:ILE:HB	1:A:190:VAL:HB	2.04	0.40
1:C:127:THR:CG2	1:C:128:LEU:N	2.84	0.40
1:D:127:THR:HG23	1:D:148:GLY:HA2	2.04	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASN:ND2	3:B:601:HOH:O	2.08	0.40
1:D:124:ASP:HB3	1:D:140:PRO:HD2	2.03	0.40
1:F:16:GLN:HG2	1:F:17:ALA:N	2.36	0.40
1:A:262:THR:OG1	3:A:603:HOH:O	2.18	0.40

All (3) 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)
3:D:669:HOH:O	3:E:671:HOH:O[1_455]	2.07	0.13
3:A:671:HOH:O	3:D:703:HOH:O[2_759]	2.09	0.11
1:B:75:LYS:HZ3	1:E:177:GLU:OE2[2_858]	1.58	0.02

## 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	279/296 (94%)	263 (94%)	11 (4%)	5 (2%)	8 3
1	B	279/296 (94%)	264 (95%)	8 (3%)	7 (2%)	5 2
1	C	279/296 (94%)	262 (94%)	12 (4%)	5 (2%)	8 3
1	D	279/296 (94%)	264 (95%)	10 (4%)	5 (2%)	8 3
1	E	262/296 (88%)	247 (94%)	12 (5%)	3 (1%)	14 8
1	F	274/296 (93%)	263 (96%)	7 (3%)	4 (2%)	10 5
All	All	1652/1776 (93%)	1563 (95%)	60 (4%)	29 (2%)	8 3

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	189	LYS
1	D	176	ASP

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	176	ASP
1	A	177	GLU
1	B	32	HIS
1	B	144	SER
1	C	89	PHE
1	C	177	GLU
1	C	188	MET
1	D	144	SER
1	F	31	ALA
1	A	89	PHE
1	A	93	LEU
1	B	33	LEU
1	B	93	LEU
1	B	177	GLU
1	D	89	PHE
1	D	177	GLU
1	E	17	ALA
1	A	31	ALA
1	F	177	GLU
1	F	128	LEU
1	D	139	MET
1	B	92	VAL
1	B	139	MET
1	A	139	MET
1	C	139	MET
1	E	143	VAL
1	F	139	MET

### 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	228/247 (92%)	210 (92%)	18 (8%)	12 8
1	B	229/247 (93%)	214 (93%)	15 (7%)	16 13
1	C	224/247 (91%)	211 (94%)	13 (6%)	20 16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	228/247 (92%)	206 (90%)	22 (10%)	8	5
1	E	215/247 (87%)	198 (92%)	17 (8%)	12	8
1	F	226/247 (92%)	208 (92%)	18 (8%)	12	8
All	All	1350/1482 (91%)	1247 (92%)	103 (8%)	13	9

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	19	ARG
1	A	44	VAL
1	A	53	ASN
1	A	70	LEU
1	A	76	LEU
1	A	78	GLN
1	A	93	LEU
1	A	97	HIS
1	A	109	LYS
1	A	118	TRP
1	A	137	HIS
1	A	152	LEU
1	A	190	VAL
1	A	201	MET
1	A	212	LEU
1	A	216	ASP
1	A	255	LEU
1	B	16	GLN
1	B	44	VAL
1	B	53	ASN
1	B	75	LYS
1	B	76	LEU
1	B	79	LYS
1	B	93	LEU
1	B	117	ILE
1	B	118	TRP
1	B	137	HIS
1	B	152	LEU
1	B	189	LYS
1	B	190	VAL
1	B	212	LEU
1	B	255	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	16	GLN
1	C	19	ARG
1	C	43	THR
1	C	76	LEU
1	C	79	LYS
1	C	93	LEU
1	C	107	THR
1	C	112	ASP
1	C	117	ILE
1	C	152	LEU
1	C	163	LYS
1	C	212	LEU
1	C	216	ASP
1	D	16	GLN
1	D	44	VAL
1	D	45	GLU
1	D	50	ILE
1	D	53	ASN
1	D	65	ASN
1	D	66	LEU
1	D	70	LEU
1	D	76	LEU
1	D	93	LEU
1	D	117	ILE
1	D	118	TRP
1	D	130	THR
1	D	137	HIS
1	D	152	LEU
1	D	175	LEU
1	D	185	GLU
1	D	189	LYS
1	D	198	ARG
1	D	212	LEU
1	D	213	SER
1	D	255	LEU
1	E	3	LYS
1	E	16	GLN
1	E	19	ARG
1	E	43	THR
1	E	44	VAL
1	E	74	GLU
1	E	76	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	93	LEU
1	E	109	LYS
1	E	112	ASP
1	E	118	TRP
1	E	139	MET
1	E	144	SER
1	E	175	LEU
1	E	189	LYS
1	E	212	LEU
1	E	255	LEU
1	F	4	THR
1	F	16	GLN
1	F	18	ARG
1	F	19	ARG
1	F	44	VAL
1	F	53	ASN
1	F	76	LEU
1	F	97	HIS
1	F	113	ASN
1	F	128	LEU
1	F	137	HIS
1	F	147	ILE
1	F	152	LEU
1	F	175	LEU
1	F	176	ASP
1	F	177	GLU
1	F	201	MET
1	F	212	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	137	HIS

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	283/296 (95%)	0.42	19 (6%) 17 21	19, 37, 72, 119	0
1	B	283/296 (95%)	0.23	16 (5%) 23 28	17, 34, 63, 104	0
1	C	283/296 (95%)	0.35	13 (4%) 32 36	22, 41, 71, 117	0
1	D	283/296 (95%)	0.22	10 (3%) 44 49	18, 36, 64, 84	0
1	E	268/296 (90%)	0.22	12 (4%) 33 37	19, 36, 64, 112	0
1	F	280/296 (94%)	0.33	14 (5%) 28 33	23, 39, 68, 119	0
All	All	1680/1776 (94%)	0.29	84 (5%) 28 33	17, 37, 69, 119	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ASN	8.2
1	F	127	THR	8.0
1	F	133	SER	5.8
1	A	66	LEU	5.7
1	B	176	ASP	5.7
1	E	14	LEU	5.2
1	A	3	LYS	5.0
1	F	53	ASN	4.8
1	E	176	ASP	4.8
1	A	176	ASP	4.7
1	F	136	ILE	4.7
1	C	175	LEU	4.5
1	B	93	LEU	4.4
1	B	128	LEU	4.3
1	A	52	ILE	4.3
1	D	176	ASP	4.3
1	A	65	ASN	4.2
1	C	128	LEU	4.1
1	D	150	GLU	4.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	117	ILE	3.6
1	A	86	GLU	3.6
1	E	17	ALA	3.5
1	A	67	ASN	3.5
1	E	69	VAL	3.4
1	D	132	PRO	3.4
1	B	117	ILE	3.4
1	F	145	LEU	3.4
1	A	214	ALA	3.3
1	A	14	LEU	3.3
1	E	177	GLU	3.1
1	C	152	LEU	3.1
1	D	53	ASN	3.1
1	D	117	ILE	2.9
1	E	16	GLN	2.9
1	D	177	GLU	2.9
1	A	93	LEU	2.8
1	F	176	ASP	2.8
1	F	135	ASN	2.8
1	A	145	LEU	2.8
1	C	72	GLY	2.7
1	C	177	GLU	2.7
1	C	87	LYS	2.6
1	D	128	LEU	2.6
1	F	128	LEU	2.6
1	B	127	THR	2.5
1	B	66	LEU	2.5
1	E	15	GLY	2.5
1	A	130	THR	2.5
1	C	132	PRO	2.4
1	C	70	LEU	2.4
1	F	18	ARG	2.4
1	C	52	ILE	2.4
1	F	152	LEU	2.4
1	A	127	THR	2.4
1	E	139	MET	2.4
1	B	92	VAL	2.4
1	B	157	GLY	2.3
1	B	70	LEU	2.3
1	D	93	LEU	2.3
1	F	52	ILE	2.3
1	A	118	TRP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	3	LYS	2.3
1	B	52	ILE	2.3
1	B	144	SER	2.3
1	E	93	LEU	2.3
1	A	43	THR	2.3
1	E	212	LEU	2.2
1	F	147	ILE	2.2
1	B	132	PRO	2.2
1	B	177	GLU	2.2
1	D	52	ILE	2.2
1	F	19	ARG	2.2
1	B	175	LEU	2.2
1	B	129	GLU	2.2
1	C	23	MET	2.2
1	C	188	MET	2.2
1	B	145	LEU	2.2
1	A	69	VAL	2.2
1	A	177	GLU	2.1
1	E	52	ILE	2.1
1	F	150	GLU	2.1
1	C	53	ASN	2.0
1	E	126	ASN	2.0
1	A	296	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MN	B	500	1/1	0.97	0.12	28,28,28,28	0
2	MN	C	501	1/1	0.97	0.11	33,33,33,33	0
2	MN	F	500	1/1	0.97	0.10	28,28,28,28	0
2	MN	A	500	1/1	0.98	0.10	24,24,24,24	0
2	MN	D	500	1/1	0.98	0.10	24,24,24,24	0
2	MN	D	501	1/1	0.98	0.13	24,24,24,24	0
2	MN	C	500	1/1	0.98	0.09	28,28,28,28	0
2	MN	F	501	1/1	0.98	0.11	27,27,27,27	0
2	MN	E	500	1/1	0.99	0.13	22,22,22,22	0
2	MN	E	501	1/1	0.99	0.14	22,22,22,22	0
2	MN	A	501	1/1	0.99	0.16	22,22,22,22	0
2	MN	B	501	1/1	0.99	0.14	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.