



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:34 AM UTC

PDB ID : 6DKT / pdb_00006dkt
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

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:

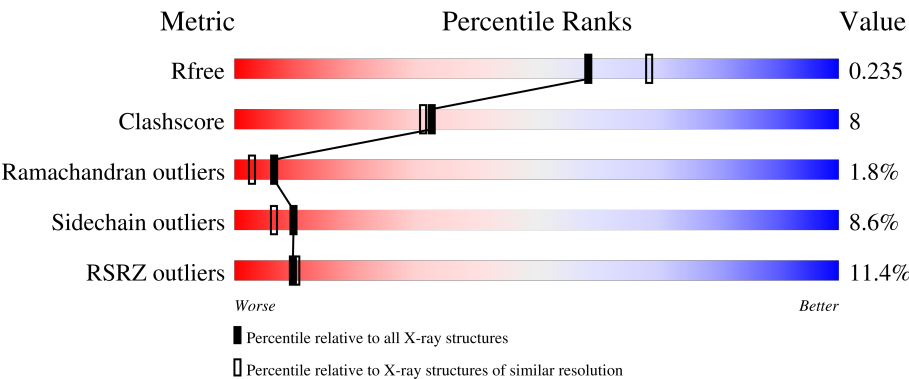
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (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 ≥ 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	13% 73%19% . .
1	B	296	10% 75%17% . .
1	C	296	12% 78%14% . .
1	D	296	10% 73%19% . .
1	E	296	9% 73%13%5%9%

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Mol	Chain	Length	Quality of chain
1	F	296	11% 76% 16% • 5%

2 Entry composition

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

- Molecule 2 is MANGANESE (II) ION (CCD ID: 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		

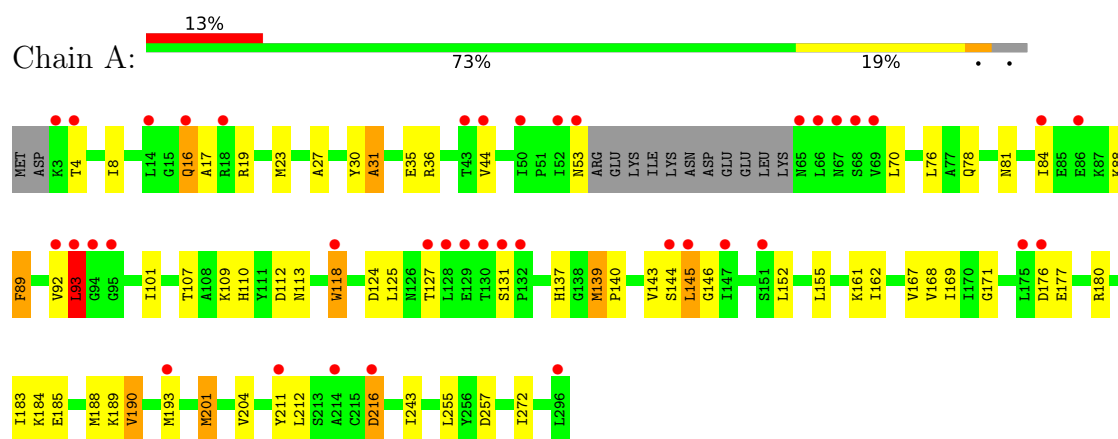
- Molecule 3 is water.

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

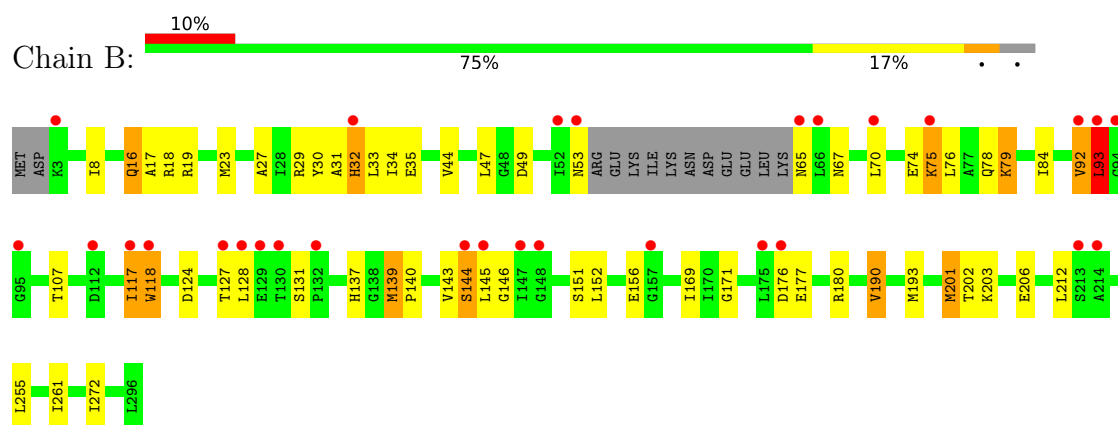
3 Residue-property plots [i](#)

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.

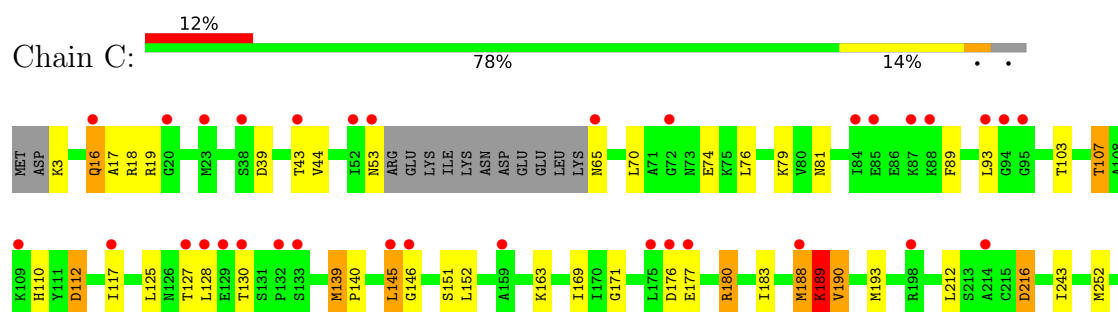
• Molecule 1: Arginase



• Molecule 1: Arginase

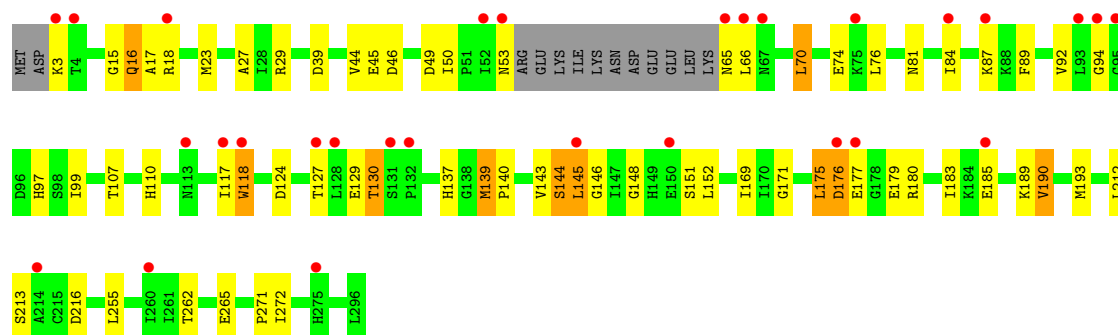
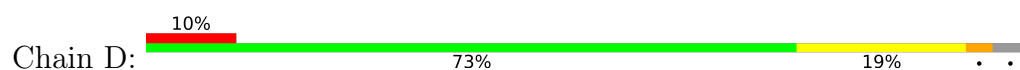


• Molecule 1: Arginase

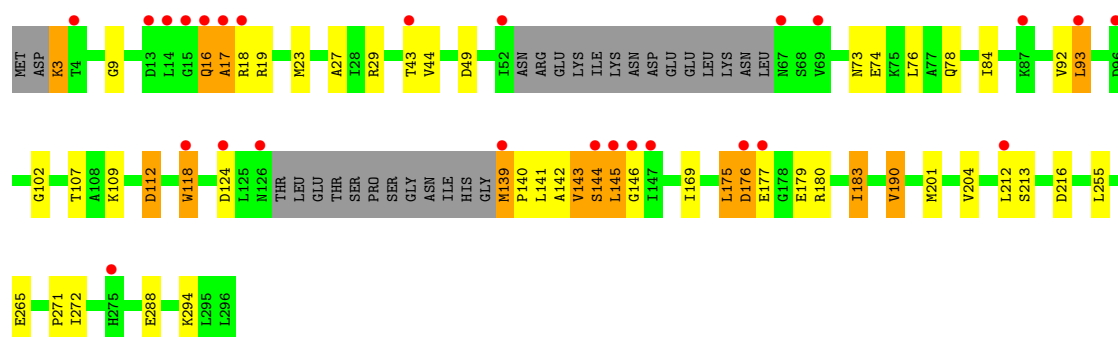
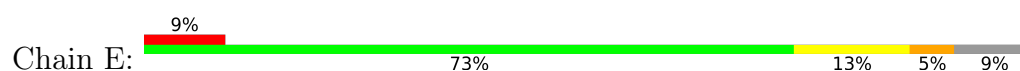




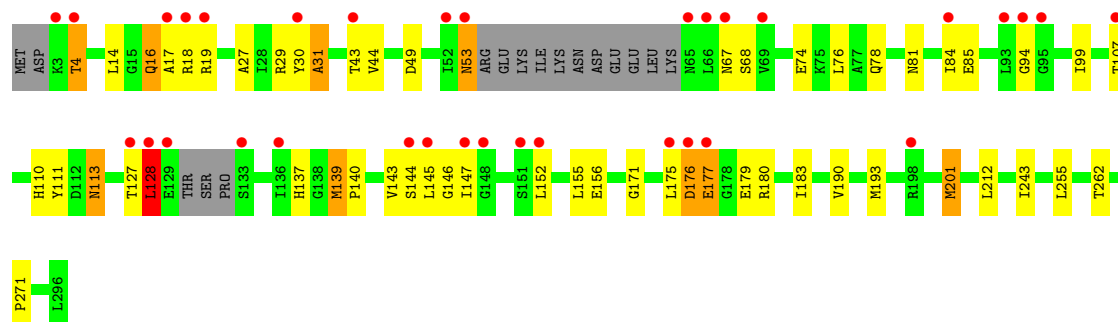
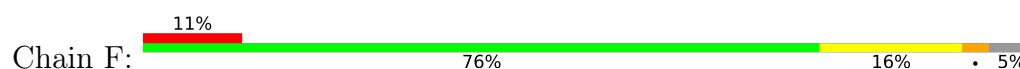
• Molecule 1: Arginase



• 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, α , β , γ	77.14Å 128.55Å 82.02Å 90.00° 112.69° 90.00°	Depositor
Resolution (Å)	47.70 – 2.08 47.70 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.70-2.08) 94.9 (47.70-2.08)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.204 , 0.231 0.207 , 0.235	Depositor DCC
R_{free} test set	2009 reflections (2.27%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25345	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.17	0/2152	0.40	1/2917 (0.0%)
1	B	0.17	0/2155	0.41	0/2919
1	C	0.15	0/2141	0.39	1/2903 (0.0%)
1	D	0.17	0/2154	0.38	1/2918 (0.0%)
1	E	0.17	0/2042	0.38	1/2765 (0.0%)
1	F	0.17	0/2133	0.37	0/2887
All	All	0.17	0/12777	0.39	4/17309 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	LEU	N-CA-C	6.25	121.06	113.38
1	A	145	LEU	N-CA-C	5.79	120.41	113.23
1	E	145	LEU	N-CA-C	5.60	120.17	113.23
1	D	145	LEU	N-CA-C	5.14	119.60	113.23

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	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2121	2052	2113	41	1
1	C	2107	2046	2082	24	0
1	D	2120	2060	2108	35	0
1	E	2011	1971	1997	30	1
1	F	2101	2035	2093	32	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	4	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	5	0
All	All	13125	12220	12497	199	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 8.

All (199) 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:B:203:LYS:NZ	3:B:605:HOH:O	2.26	0.69
1:D:65:ASN:N	3:D:606:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:SER:OG	3:B:603:HOH:O	2.12	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
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:A:169:ILE:HD11	1:A:188:MET:HE1	1.80	0.63
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: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:143:VAL:C	1:F:144:SER:HG	2.02	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:93:LEU:C	1:A:93:LEU:HD23	2.35	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
1:A:169:ILE:CD1	1:A:188:MET:HE1	2.41	0.51
1:B:118:TRP:CH2	1:B:124:ASP:HB2	2.45	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:A:139:MET:N	1:A:140:PRO:CD	2.74	0.50
1:C:193:MET:HE1	1:C:243:ILE:HG13	1.94	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:F:201:MET:HE3	1:F:201:MET:HA	1.95	0.48
1:C:252:MET:HE3	1:C:290:LEU:HB2	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:142:ALA:C	1:E:143:VAL:O	2.57	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:A:30:TYR:O	1:A:31:ALA:HB3	2.15	0.47
1:F:74:GLU:HG3	1:F:155:LEU:HD11	1.97	0.47
1:F:193:MET:HE1	1:F:243:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:23:MET:HE1	1:D:272:ILE:HD11	1.96	0.47
1:A:8:ILE:O	1:A:92:VAL:O	2.33	0.47
1:A:167:VAL:CG1	1:A:188:MET:HE3	2.45	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
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:E:23:MET:HE1	1:E:272:ILE:HD11	1.97	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:A:188:MET:HE2	1:A:188:MET:HB3	1.83	0.45
1:B:93:LEU:HD23	1:B:93:LEU:C	2.42	0.45
1:C:169:ILE:HB	1:C:190:VAL:HB	1.99	0.45
1:A:201:MET:HE2	1:A:204:VAL:HB	1.97	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:B:23:MET:HE3	1:B:272:ILE:HG12	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ASP:OD1	1:D:216:ASP:N	2.47	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:B:201:MET:HE3	1:B:201:MET:HA	2.01	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:201:MET:HE3	1:E:204:VAL:HB	2.01	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
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:A:201:MET:HE3	1:A:201:MET:HA	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: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:A:193:MET:HE1	1:A:243:ILE:HG13	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:23:MET:HE1	1:A:272:ILE:HD11	2.03	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
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

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%)	6	3
1	B	279/296 (94%)	264 (95%)	8 (3%)	7 (2%)	4	1
1	C	279/296 (94%)	262 (94%)	12 (4%)	5 (2%)	6	3
1	D	279/296 (94%)	264 (95%)	10 (4%)	5 (2%)	6	3
1	E	262/296 (88%)	247 (94%)	12 (5%)	3 (1%)	11	7
1	F	274/296 (93%)	263 (96%)	7 (3%)	4 (2%)	8	4
All	All	1652/1776 (93%)	1563 (95%)	60 (4%)	29 (2%)	6	3

All (29) Ramachandran outliers are listed below:

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

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%)	211 (92%)	17 (8%)	12	9
1	B	229/247 (93%)	212 (93%)	17 (7%)	13	9
1	C	224/247 (91%)	203 (91%)	21 (9%)	8	5
1	D	228/247 (92%)	206 (90%)	22 (10%)	8	5
1	E	215/247 (87%)	196 (91%)	19 (9%)	9	6
1	F	226/247 (92%)	206 (91%)	20 (9%)	9	6
All	All	1350/1482 (91%)	1234 (91%)	116 (9%)	10	6

All (116) 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	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	18	ARG
1	B	19	ARG
1	B	44	VAL
1	B	53	ASN

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Mol	Chain	Res	Type
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	190	VAL
1	B	201	MET
1	B	212	LEU
1	B	255	LEU
1	C	16	GLN
1	C	18	ARG
1	C	19	ARG
1	C	43	THR
1	C	44	VAL
1	C	53	ASN
1	C	74	GLU
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	180	ARG
1	C	189	LYS
1	C	190	VAL
1	C	212	LEU
1	C	216	ASP
1	C	255	LEU
1	D	16	GLN
1	D	18	ARG
1	D	44	VAL
1	D	45	GLU
1	D	50	ILE
1	D	53	ASN
1	D	66	LEU
1	D	70	LEU
1	D	74	GLU

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Mol	Chain	Res	Type
1	D	76	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	190	VAL
1	D	212	LEU
1	D	213	SER
1	D	255	LEU
1	E	3	LYS
1	E	16	GLN
1	E	18	ARG
1	E	19	ARG
1	E	43	THR
1	E	44	VAL
1	E	74	GLU
1	E	76	LEU
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	183	ILE
1	E	190	VAL
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	113	ASN
1	F	128	LEU
1	F	137	HIS

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Mol	Chain	Res	Type
1	F	147	ILE
1	F	152	LEU
1	F	175	LEU
1	F	176	ASP
1	F	177	GLU
1	F	180	ARG
1	F	190	VAL
1	F	201	MET
1	F	212	LEU
1	F	255	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	B	113	ASN
1	D	137	HIS
1	E	154	ASN
1	F	149	HIS
1	F	275	HIS

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 oligosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/296 (95%)	0.69	39 (13%) 6 7	21, 41, 77, 129	0
1	B	283/296 (95%)	0.57	29 (10%) 12 13	19, 38, 71, 109	0
1	C	283/296 (95%)	0.77	35 (12%) 8 8	24, 46, 79, 130	0
1	D	283/296 (95%)	0.53	29 (10%) 12 13	20, 40, 69, 93	0
1	E	268/296 (90%)	0.52	26 (9%) 13 14	21, 40, 70, 124	0
1	F	280/296 (94%)	0.64	33 (11%) 9 9	25, 43, 75, 130	0
All	All	1680/1776 (94%)	0.62	191 (11%) 10 10	19, 41, 76, 130	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	LEU	7.5
1	C	132	PRO	6.7
1	B	93	LEU	6.1
1	F	127	THR	5.8
1	C	175	LEU	5.7
1	D	176	ASP	5.6
1	A	52	ILE	5.5
1	B	129	GLU	5.5
1	C	117	ILE	5.1
1	E	14	LEU	5.0
1	F	129	GLU	5.0
1	B	176	ASP	4.9
1	A	3	LYS	4.6
1	B	144	SER	4.5
1	E	176	ASP	4.5
1	A	66	LEU	4.5
1	B	117	ILE	4.4
1	A	93	LEU	4.4
1	F	53	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	128	LEU	4.4
1	F	145	LEU	4.4
1	D	53	ASN	4.3
1	A	176	ASP	4.3
1	D	128	LEU	4.2
1	E	16	GLN	4.2
1	B	175	LEU	4.2
1	D	93	LEU	4.2
1	C	65	ASN	4.2
1	E	17	ALA	4.1
1	F	176	ASP	4.0
1	F	136	ILE	4.0
1	C	53	ASN	4.0
1	B	52	ILE	4.0
1	A	129	GLU	3.9
1	B	157	GLY	3.9
1	A	53	ASN	3.8
1	A	4	THR	3.8
1	A	69	VAL	3.8
1	E	15	GLY	3.8
1	F	177	GLU	3.8
1	B	130	THR	3.8
1	D	117	ILE	3.7
1	B	3	LYS	3.7
1	A	132	PRO	3.7
1	A	130	THR	3.7
1	C	128	LEU	3.7
1	B	65	ASN	3.7
1	F	144	SER	3.7
1	B	53	ASN	3.6
1	F	133	SER	3.6
1	C	23	MET	3.6
1	E	126	ASN	3.6
1	A	145	LEU	3.5
1	B	145	LEU	3.5
1	D	3	LYS	3.5
1	B	127	THR	3.4
1	D	52	ILE	3.4
1	F	93	LEU	3.4
1	C	94	GLY	3.3
1	E	93	LEU	3.3
1	D	150	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	177	GLU	3.2
1	A	14	LEU	3.2
1	B	94	GLY	3.2
1	B	213	SER	3.2
1	A	214	ALA	3.2
1	A	175	LEU	3.2
1	E	147	ILE	3.1
1	F	84	ILE	3.1
1	A	86	GLU	3.1
1	A	144	SER	3.1
1	E	144	SER	3.1
1	E	18	ARG	3.1
1	B	66	LEU	3.1
1	A	68	SER	3.1
1	A	65	ASN	3.0
1	F	147	ILE	3.0
1	B	92	VAL	3.0
1	C	177	GLU	3.0
1	E	52	ILE	3.0
1	F	66	LEU	2.9
1	F	94	GLY	2.9
1	F	95	GLY	2.9
1	E	69	VAL	2.8
1	D	65	ASN	2.8
1	C	93	LEU	2.8
1	A	211	TYR	2.8
1	A	84	ILE	2.8
1	A	127	THR	2.8
1	E	139	MET	2.7
1	A	43	THR	2.7
1	F	18	ARG	2.7
1	A	118	TRP	2.7
1	C	176	ASP	2.7
1	C	95	GLY	2.7
1	E	87	LYS	2.7
1	B	70	LEU	2.7
1	C	188	MET	2.7
1	B	147	ILE	2.7
1	E	13	ASP	2.7
1	F	19	ARG	2.7
1	E	118	TRP	2.7
1	C	16	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	214	ALA	2.6
1	D	127	THR	2.6
1	D	132	PRO	2.6
1	F	198	ARG	2.6
1	A	151	SER	2.6
1	D	67	ASN	2.5
1	C	133	SER	2.5
1	C	129	GLU	2.5
1	E	124	ASP	2.5
1	E	4	THR	2.5
1	B	95	GLY	2.5
1	C	52	ILE	2.5
1	E	43	THR	2.5
1	A	128	LEU	2.5
1	D	177	GLU	2.4
1	C	127	THR	2.4
1	F	3	LYS	2.4
1	F	175	LEU	2.4
1	B	148	GLY	2.4
1	C	72	GLY	2.4
1	A	67	ASN	2.4
1	D	118	TRP	2.4
1	C	43	THR	2.4
1	C	145	LEU	2.4
1	E	146	GLY	2.4
1	F	52	ILE	2.4
1	C	109	LYS	2.4
1	D	275	HIS	2.4
1	A	50	ILE	2.4
1	C	38	SER	2.4
1	F	151	SER	2.4
1	B	132	PRO	2.4
1	E	275	HIS	2.4
1	D	66	LEU	2.3
1	B	112	ASP	2.3
1	D	131	SER	2.3
1	F	4	THR	2.3
1	C	214	ALA	2.3
1	A	94	GLY	2.3
1	F	152	LEU	2.3
1	D	18	ARG	2.3
1	E	212	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	32	HIS	2.3
1	F	107	THR	2.3
1	C	198	ARG	2.3
1	D	75	LYS	2.3
1	D	260	ILE	2.2
1	F	69	VAL	2.2
1	E	67	ASN	2.2
1	F	67	ASN	2.2
1	A	95	GLY	2.2
1	C	275	HIS	2.2
1	B	118	TRP	2.2
1	C	88	LYS	2.2
1	C	130	THR	2.2
1	E	145	LEU	2.2
1	D	113	ASN	2.2
1	F	43	THR	2.2
1	A	44	VAL	2.2
1	D	95	GLY	2.2
1	D	185	GLU	2.2
1	F	30	TYR	2.2
1	B	75	LYS	2.2
1	C	272	ILE	2.1
1	C	146	GLY	2.1
1	D	214	ALA	2.1
1	F	17	ALA	2.1
1	D	145	LEU	2.1
1	A	147	ILE	2.1
1	D	87	LYS	2.1
1	A	131	SER	2.1
1	A	193	MET	2.1
1	F	65	ASN	2.1
1	A	16	GLN	2.1
1	D	84	ILE	2.1
1	F	148	GLY	2.1
1	A	296	LEU	2.1
1	A	216	ASP	2.1
1	E	96	ASP	2.1
1	C	84	ILE	2.1
1	C	87	LYS	2.1
1	A	92	VAL	2.1
1	C	85	GLU	2.0
1	C	20	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	94	GLY	2.0
1	C	159	ALA	2.0
1	A	18	ARG	2.0
1	D	4	THR	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 oligosaccharides 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, 95th 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	A	501	1/1	0.96	0.05	22,22,22,22	0
2	MN	B	500	1/1	0.97	0.06	28,28,28,28	0
2	MN	D	501	1/1	0.97	0.04	24,24,24,24	0
2	MN	E	500	1/1	0.97	0.04	22,22,22,22	0
2	MN	F	500	1/1	0.97	0.05	28,28,28,28	0
2	MN	A	500	1/1	0.98	0.04	24,24,24,24	0
2	MN	B	501	1/1	0.98	0.05	24,24,24,24	0
2	MN	C	501	1/1	0.98	0.05	33,33,33,33	0
2	MN	D	500	1/1	0.99	0.02	24,24,24,24	0
2	MN	E	501	1/1	0.99	0.04	22,22,22,22	0
2	MN	C	500	1/1	0.99	0.03	28,28,28,28	0
2	MN	F	501	1/1	0.99	0.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.