Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 08:01 AM EDT

PDB ID	:	6X60
Title	:	ClpP2 from Chlamydia trachomatis with resolved handle loop
Authors	:	Azadmanesh, J.; Struble, L.R.; Seleem, M.A.; Ouellette, S.; Conda-Sheridan, M.; Borgstahl, G.E.O.
Deposited on	:	2020-05-27
Resolution	:	2.81 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:

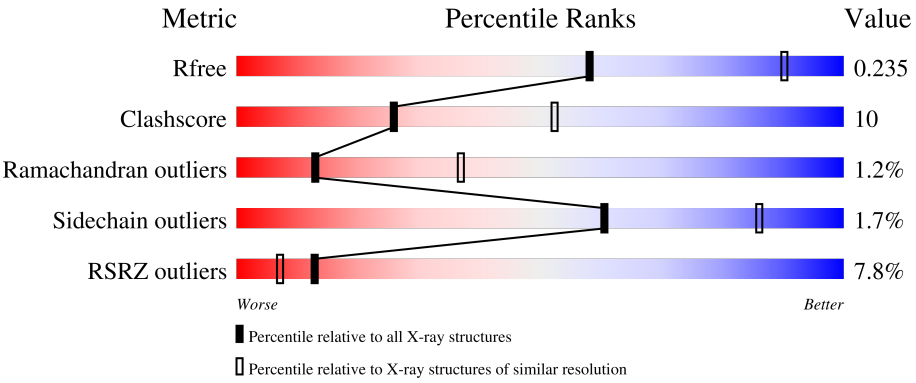
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	203	7% 73% 18% • 8%
1	B	203	7% 72% 21% • 5%
1	C	203	7% 71% 19% • 7%
1	D	203	6% 73% 17% • 8%
1	E	203	10% 74% 20% • 5%

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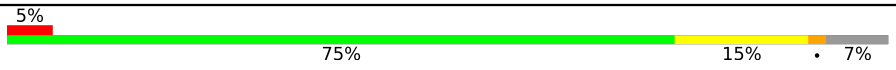
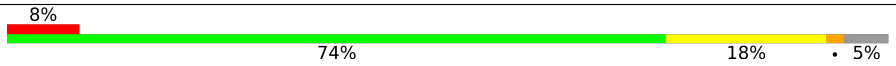
Mol	Chain	Length	Quality of chain
1	F	203	
1	G	203	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10106 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 ATP-dependent Clp protease proteolytic subunit 2.

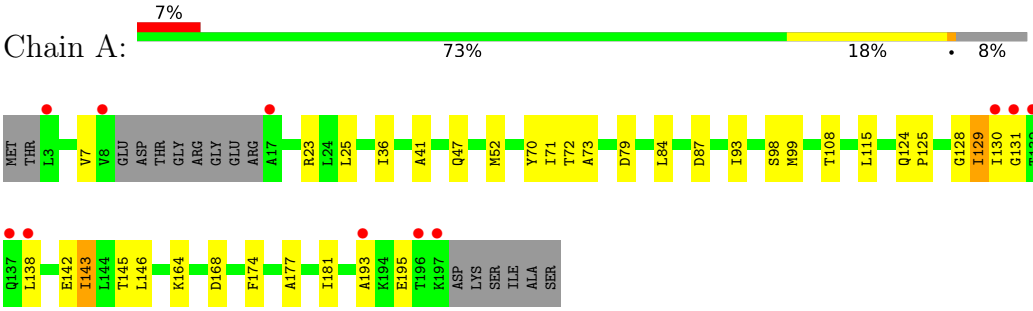
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	0
			1421	906	233	272	10			
1	B	192	Total	C	N	O	S	0	0	0
			1464	930	242	282	10			
1	C	189	Total	C	N	O	S	0	0	0
			1438	916	236	276	10			
1	D	187	Total	C	N	O	S	0	0	0
			1419	904	232	273	10			
1	E	193	Total	C	N	O	S	0	0	0
			1468	932	243	283	10			
1	F	188	Total	C	N	O	S	0	0	0
			1432	912	237	273	10			
1	G	192	Total	C	N	O	S	0	0	0
			1464	930	242	282	10			

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.

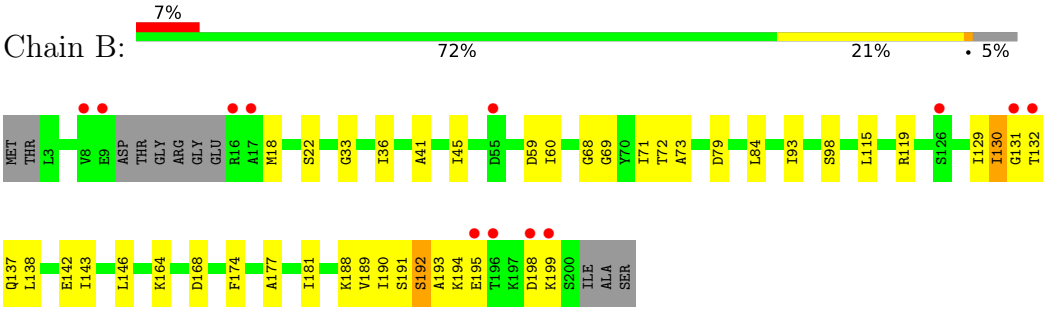
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain A:



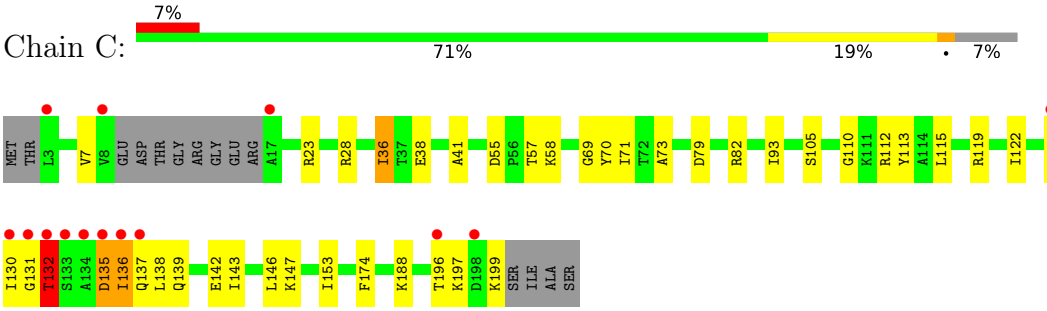
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain B:



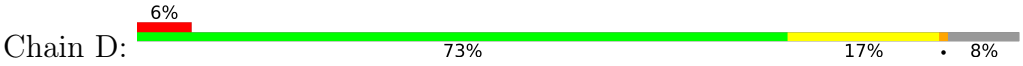
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

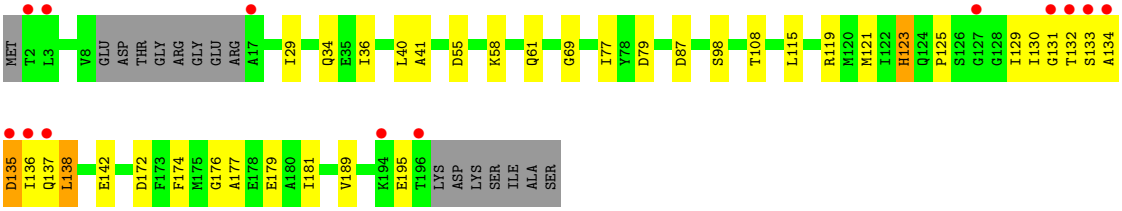
Chain C:



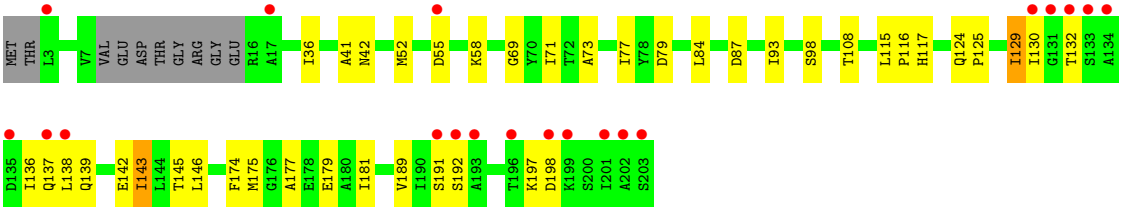
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain D:

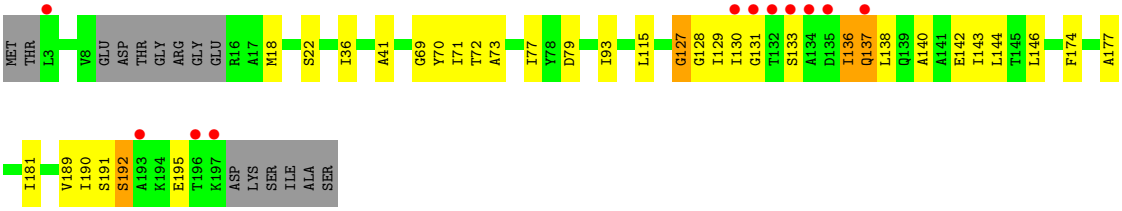




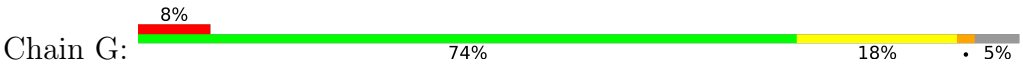
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

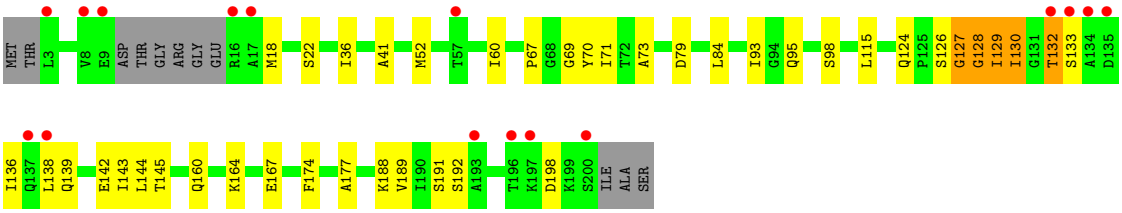


• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.71Å 147.04Å 97.06Å 90.00° 128.25° 90.00°	Depositor
Resolution (Å)	28.16 – 2.81 28.16 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.3 (28.16-2.81) 96.3 (28.16-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.18rc2_3794	Depositor
R, R_{free}	0.198 , 0.235 0.198 , 0.235	Depositor DCC
R_{free} test set	2029 reflections (6.03%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10106	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.28	0/1440	0.55	0/1944
1	B	0.28	0/1483	0.53	0/2000
1	C	0.29	0/1457	0.57	1/1966 (0.1%)
1	D	0.27	0/1438	0.55	1/1943 (0.1%)
1	E	0.28	0/1487	0.53	0/2004
1	F	0.28	0/1451	0.53	0/1958
1	G	0.33	0/1483	0.58	2/2000 (0.1%)
All	All	0.29	0/10239	0.55	4/13815 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	F	0	1
All	All	0	3

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	C	135	ASP	CB-CG-OD1	9.62	126.96	118.30
1	G	129	ILE	CA-CB-CG2	-6.42	98.06	110.90
1	G	129	ILE	CG1-CB-CG2	5.54	123.58	111.40
1	D	123	HIS	C-N-CA	5.33	135.03	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	135	ASP	Peptide
1	D	135	ASP	Peptide
1	F	137	GLN	Peptide

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	1421	0	1460	32	0
1	B	1464	0	1501	41	0
1	C	1438	0	1477	40	0
1	D	1419	0	1454	27	0
1	E	1468	0	1507	31	0
1	F	1432	0	1473	31	0
1	G	1464	0	1501	42	0
All	All	10106	0	10373	215	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 10.

All (215) 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:G:71:ILE:H	1:G:130:ILE:HG21	1.24	1.01
1:C:38:GLU:HG2	1:C:132:THR:HA	1.49	0.90
1:G:70:TYR:HA	1:G:130:ILE:HG13	1.51	0.89
1:B:188:LYS:HD3	1:B:195:GLU:HG2	1.54	0.89
1:G:71:ILE:HB	1:G:130:ILE:HG21	1.54	0.87
1:F:130:ILE:HG21	1:F:138:LEU:HD23	1.60	0.83
1:G:71:ILE:H	1:G:130:ILE:CG2	1.90	0.83
1:B:71:ILE:H	1:B:130:ILE:HG13	1.43	0.82
1:B:71:ILE:N	1:B:130:ILE:HG13	1.95	0.81
1:G:71:ILE:N	1:G:130:ILE:HG21	1.97	0.79
1:B:131:GLY:HA3	1:B:136:ILE:HB	1.66	0.77
1:C:128:GLY:O	1:C:147:LYS:NZ	2.19	0.76
1:F:136:ILE:HD12	1:F:136:ILE:H	1.51	0.75
1:C:70:TYR:HB3	1:C:131:GLY:HA2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:CG	1:C:132:THR:HA	2.20	0.72
1:B:115:LEU:HD23	1:E:79:ASP:HB3	1.74	0.70
1:F:127:GLY:O	1:F:129:ILE:N	2.24	0.70
1:A:130:ILE:HG22	1:A:136:ILE:HG22	1.74	0.69
1:B:59:ASP:OD2	1:B:199:LYS:NZ	2.20	0.69
1:C:129:ILE:HD13	1:C:130:ILE:HG13	1.73	0.68
1:D:115:LEU:HD13	1:G:79:ASP:HB3	1.75	0.68
1:G:71:ILE:CB	1:G:130:ILE:HG21	2.22	0.68
1:B:181:ILE:HD11	1:B:189:VAL:HG23	1.76	0.68
1:D:172:ASP:OD2	1:G:139:GLN:NE2	2.28	0.67
1:F:70:TYR:CD1	1:F:131:GLY:HA3	2.31	0.66
1:G:127:GLY:C	1:G:129:ILE:H	1.99	0.66
1:C:79:ASP:HB3	1:E:115:LEU:HD23	1.79	0.65
1:B:93:ILE:HG12	1:B:115:LEU:HD22	1.78	0.64
1:E:177:ALA:HB1	1:E:189:VAL:HG22	1.78	0.63
1:G:133:SER:HA	1:G:136:ILE:HG23	1.81	0.63
1:C:130:ILE:HG12	1:C:136:ILE:HD12	1.81	0.62
1:G:36:ILE:HB	1:G:69:GLY:HA3	1.80	0.62
1:B:79:ASP:HB3	1:G:115:LEU:HD23	1.83	0.61
1:B:142:GLU:HG3	1:G:174:PHE:CD1	2.35	0.60
1:E:139:GLN:O	1:E:143:ILE:HG13	2.01	0.60
1:C:130:ILE:HD13	1:C:136:ILE:HB	1.82	0.59
1:G:126:SER:O	1:G:128:GLY:N	2.35	0.59
1:A:79:ASP:HB3	1:C:115:LEU:HD23	1.84	0.59
1:B:132:THR:CG2	1:G:67:PRO:HB3	2.33	0.59
1:E:98:SER:OG	1:E:124:GLN:NE2	2.36	0.59
1:A:115:LEU:HD23	1:F:79:ASP:HB3	1.84	0.59
1:A:129:ILE:HG21	1:A:143:ILE:HD13	1.83	0.58
1:B:136:ILE:HD12	1:B:138:LEU:H	1.68	0.58
1:C:136:ILE:HG23	1:C:137:GLN:H	1.67	0.58
1:B:36:ILE:HB	1:B:69:GLY:HA3	1.85	0.58
1:B:195:GLU:OE1	1:B:195:GLU:N	2.37	0.58
1:B:132:THR:HG23	1:G:95:GLN:HE22	1.68	0.58
1:B:131:GLY:HA3	1:B:136:ILE:CB	2.33	0.58
1:C:93:ILE:HG12	1:C:115:LEU:HD22	1.85	0.58
1:A:93:ILE:HG12	1:A:115:LEU:HD22	1.86	0.57
1:E:93:ILE:HG12	1:E:115:LEU:HD22	1.86	0.57
1:A:7:VAL:HG11	1:A:23:ARG:HB2	1.87	0.56
1:E:197:LYS:HG2	1:E:198:ASP:H	1.70	0.56
1:B:132:THR:HG23	1:G:67:PRO:HB3	1.87	0.56
1:E:138:LEU:HD21	1:E:143:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ILE:HG12	1:F:115:LEU:HD22	1.87	0.56
1:C:129:ILE:H	1:C:129:ILE:HD12	1.70	0.56
1:C:110:GLY:HA2	1:C:188:LYS:HZ2	1.70	0.56
1:C:197:LYS:HG2	1:C:199:LYS:H	1.72	0.55
1:E:129:ILE:HD13	1:E:136:ILE:HG23	1.88	0.55
1:F:70:TYR:HB3	1:F:130:ILE:O	2.06	0.54
1:C:136:ILE:HG12	1:C:138:LEU:H	1.72	0.54
1:E:138:LEU:HD21	1:E:143:ILE:HG23	1.89	0.54
1:F:70:TYR:CE1	1:F:131:GLY:HA3	2.42	0.54
1:B:129:ILE:O	1:B:136:ILE:HG21	2.08	0.54
1:D:181:ILE:HD11	1:D:189:VAL:HG23	1.90	0.54
1:D:142:GLU:HG3	1:F:174:PHE:CD1	2.44	0.53
1:B:191:SER:H	1:B:194:LYS:HE2	1.74	0.53
1:D:130:ILE:HB	1:D:138:LEU:HD22	1.89	0.53
1:F:129:ILE:HG23	1:F:136:ILE:HG23	1.90	0.53
1:B:190:ILE:HA	1:B:194:LYS:HE3	1.90	0.53
1:F:136:ILE:HG22	1:F:137:GLN:H	1.74	0.53
1:F:140:ALA:O	1:F:143:ILE:HG13	2.09	0.53
1:B:131:GLY:CA	1:B:136:ILE:HB	2.38	0.53
1:D:132:THR:HG21	1:D:137:GLN:NE2	2.24	0.53
1:G:127:GLY:O	1:G:129:ILE:N	2.42	0.53
1:D:133:SER:O	1:D:136:ILE:HG22	2.10	0.52
1:D:131:GLY:HA2	1:D:135:ASP:HA	1.92	0.52
1:C:71:ILE:HG21	1:C:146:LEU:HB3	1.92	0.51
1:F:36:ILE:HB	1:F:69:GLY:HA3	1.92	0.51
1:D:36:ILE:HB	1:D:69:GLY:HA3	1.91	0.51
1:A:142:GLU:HG3	1:C:174:PHE:CD2	2.45	0.51
1:B:72:THR:HG23	1:B:130:ILE:HD11	1.93	0.51
1:D:29:ILE:HG12	1:D:61:GLN:HB2	1.93	0.51
1:E:116:PRO:HG3	1:E:191:SER:HB3	1.93	0.51
1:G:130:ILE:O	1:G:130:ILE:HG22	2.09	0.51
1:B:41:ALA:HB2	1:B:73:ALA:HB1	1.93	0.50
1:B:119:ARG:CZ	1:E:145:THR:HG21	2.41	0.50
1:G:98:SER:OG	1:G:124:GLN:HA	2.11	0.50
1:C:41:ALA:HB2	1:C:73:ALA:HB1	1.92	0.50
1:G:71:ILE:N	1:G:130:ILE:CG2	2.66	0.50
1:G:188:LYS:HA	1:G:198:ASP:HB3	1.94	0.50
1:A:70:TYR:CD1	1:A:128:GLY:HA2	2.46	0.50
1:C:110:GLY:HA2	1:C:188:LYS:NZ	2.25	0.50
1:C:82:ARG:O	1:E:192:SER:HA	2.12	0.50
1:D:177:ALA:HB1	1:D:189:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ALA:HB2	1:F:73:ALA:HB1	1.94	0.50
1:C:130:ILE:CD1	1:C:136:ILE:HB	2.42	0.49
1:F:190:ILE:HA	1:F:195:GLU:OE1	2.12	0.49
1:G:127:GLY:C	1:G:129:ILE:N	2.64	0.49
1:G:164:LYS:HA	1:G:167:GLU:HG2	1.94	0.49
1:D:87:ASP:HA	1:D:108:THR:HG21	1.93	0.49
1:E:181:ILE:HD11	1:E:189:VAL:HG23	1.93	0.49
1:B:142:GLU:HG3	1:G:174:PHE:HD1	1.78	0.49
1:B:191:SER:O	1:B:192:SER:OG	2.26	0.49
1:B:71:ILE:HG21	1:B:146:LEU:HB3	1.94	0.49
1:G:71:ILE:HB	1:G:130:ILE:CG2	2.33	0.48
1:A:138:LEU:HD23	1:A:143:ILE:HG12	1.96	0.48
1:D:34:GLN:HG3	1:D:40:LEU:HD22	1.95	0.48
1:A:129:ILE:HG13	1:A:136:ILE:HD13	1.95	0.48
1:A:98:SER:CB	1:A:125:PRO:HD3	2.43	0.48
1:D:98:SER:HB2	1:D:125:PRO:HD3	1.95	0.47
1:G:133:SER:HA	1:G:136:ILE:CG2	2.43	0.47
1:C:129:ILE:H	1:C:129:ILE:CD1	2.25	0.47
1:E:130:ILE:HG23	1:E:138:LEU:HD22	1.96	0.47
1:F:138:LEU:CD1	1:F:142:GLU:HB3	2.44	0.47
1:G:60:ILE:HD12	1:G:84:LEU:HD13	1.97	0.47
1:A:72:THR:HG21	1:A:130:ILE:HG13	1.95	0.47
1:G:177:ALA:HB1	1:G:189:VAL:HG22	1.96	0.47
1:A:70:TYR:CG	1:A:131:GLY:HA2	2.50	0.47
1:C:142:GLU:HG3	1:E:174:PHE:CD1	2.49	0.47
1:C:113:TYR:OH	1:C:196:THR:O	2.29	0.47
1:B:132:THR:CG2	1:G:95:GLN:HE22	2.27	0.47
1:F:129:ILE:CG2	1:F:131:GLY:H	2.28	0.47
1:B:45:ILE:HD13	1:G:93:ILE:HG21	1.97	0.46
1:E:36:ILE:HB	1:E:69:GLY:HA3	1.98	0.46
1:E:71:ILE:HG21	1:E:146:LEU:HB3	1.97	0.46
1:G:41:ALA:HB2	1:G:73:ALA:HB1	1.97	0.46
1:B:190:ILE:HG22	1:B:195:GLU:OE1	2.16	0.46
1:D:41:ALA:HA	1:D:77:ILE:HD11	1.97	0.46
1:D:142:GLU:HG3	1:F:174:PHE:HD1	1.80	0.46
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.47	0.46
1:D:79:ASP:HB3	1:F:115:LEU:HD23	1.98	0.45
1:A:52:MET:HB2	1:A:84:LEU:HD22	1.98	0.45
1:E:55:ASP:OD2	1:E:58:LYS:HE2	2.15	0.45
1:D:121:MET:SD	1:D:123:HIS:HB3	2.56	0.45
1:E:87:ASP:HA	1:E:108:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:MET:HB2	1:E:84:LEU:HD22	1.98	0.45
1:F:18:MET:HB2	1:F:22:SER:HB2	1.98	0.45
1:E:41:ALA:HB2	1:E:73:ALA:HB1	1.99	0.45
1:B:68:GLY:HA2	1:B:98:SER:HB3	1.99	0.45
1:F:177:ALA:O	1:F:181:ILE:HG13	2.16	0.45
1:E:143:ILE:HG13	1:E:143:ILE:H	1.61	0.44
1:F:130:ILE:HG23	1:F:131:GLY:N	2.31	0.44
1:A:98:SER:HB2	1:A:125:PRO:HD3	2.00	0.44
1:C:36:ILE:HB	1:C:69:GLY:HA3	1.99	0.44
1:A:142:GLU:HG3	1:C:174:PHE:HD2	1.83	0.44
1:F:138:LEU:HA	1:F:138:LEU:HD13	1.58	0.44
1:F:138:LEU:HD12	1:F:142:GLU:HB3	1.99	0.44
1:B:129:ILE:HG23	1:B:143:ILE:HD13	2.00	0.44
1:D:174:PHE:HB2	1:G:142:GLU:OE1	2.17	0.44
1:A:98:SER:OG	1:A:125:PRO:HD3	2.18	0.43
1:A:177:ALA:O	1:A:181:ILE:HG13	2.18	0.43
1:D:131:GLY:HA2	1:D:134:ALA:O	2.19	0.43
1:G:126:SER:O	1:G:127:GLY:C	2.55	0.43
1:G:160:GLN:OE1	1:G:164:LYS:HD3	2.18	0.43
1:A:129:ILE:CG1	1:A:136:ILE:HD13	2.48	0.43
1:A:129:ILE:H	1:A:129:ILE:HG12	1.53	0.43
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.82	0.43
1:B:177:ALA:HB1	1:B:189:VAL:HG22	2.01	0.43
1:D:55:ASP:OD2	1:D:58:LYS:HE2	2.19	0.43
1:E:41:ALA:HA	1:E:77:ILE:HD11	2.00	0.43
1:B:33:GLY:O	1:E:42:ASN:ND2	2.50	0.43
1:B:164:LYS:HE3	1:B:168:ASP:OD2	2.19	0.43
1:C:132:THR:OG1	1:C:135:ASP:OD1	2.25	0.43
1:C:142:GLU:O	1:C:146:LEU:HG	2.19	0.42
1:D:138:LEU:HD12	1:D:138:LEU:HA	1.83	0.42
1:E:132:THR:HG21	1:E:137:GLN:OE1	2.19	0.42
1:B:133:SER:H	1:B:137:GLN:HG2	1.84	0.42
1:C:132:THR:HG23	1:C:135:ASP:O	2.20	0.42
1:D:98:SER:CB	1:D:125:PRO:HD3	2.50	0.42
1:G:143:ILE:HG22	1:G:144:LEU:N	2.33	0.42
1:G:130:ILE:O	1:G:138:LEU:CD2	2.68	0.42
1:C:55:ASP:OD1	1:C:58:LYS:HE2	2.18	0.42
1:C:105:SER:HA	1:C:112:ARG:HD2	2.01	0.42
1:D:176:GLY:N	1:D:179:GLU:OE1	2.26	0.42
1:E:138:LEU:CD2	1:E:143:ILE:HG12	2.50	0.42
1:A:36:ILE:HD12	1:A:99:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLN:O	1:C:143:ILE:HG13	2.20	0.42
1:F:191:SER:O	1:F:192:SER:OG	2.29	0.42
1:B:18:MET:HB2	1:B:22:SER:HB2	2.00	0.42
1:B:36:ILE:HG12	1:B:68:GLY:O	2.20	0.42
1:B:60:ILE:HD12	1:B:84:LEU:HD13	2.02	0.42
1:F:71:ILE:HG21	1:F:146:LEU:HB3	2.01	0.42
1:G:191:SER:O	1:G:192:SER:OG	2.29	0.42
1:C:28:ARG:HD2	1:C:58:LYS:HE3	2.01	0.41
1:B:193:ALA:HB1	1:B:198:ASP:CB	2.50	0.41
1:A:41:ALA:HB2	1:A:73:ALA:HB1	2.02	0.41
1:A:70:TYR:HD1	1:A:128:GLY:HA2	1.86	0.41
1:D:119:ARG:CZ	1:G:145:THR:HG21	2.50	0.41
1:A:71:ILE:HG21	1:A:146:LEU:HB3	2.01	0.41
1:A:164:LYS:HE3	1:A:168:ASP:OD2	2.20	0.41
1:A:124:GLN:NE2	1:A:128:GLY:O	2.54	0.41
1:D:36:ILE:HA	1:D:40:LEU:HD23	2.03	0.41
1:G:71:ILE:CA	1:G:130:ILE:HG21	2.50	0.41
1:C:130:ILE:CG2	1:C:131:GLY:N	2.84	0.41
1:F:143:ILE:HD12	1:F:144:LEU:N	2.35	0.41
1:B:174:PHE:HB2	1:E:142:GLU:OE1	2.21	0.41
1:A:25:LEU:HD13	1:A:47:GLN:HE21	1.85	0.41
1:A:87:ASP:HA	1:A:108:THR:HG21	2.03	0.41
1:C:55:ASP:OD2	1:C:57:THR:HG22	2.20	0.41
1:C:135:ASP:OD1	1:C:135:ASP:O	2.38	0.41
1:C:136:ILE:HG12	1:C:137:GLN:N	2.36	0.41
1:F:72:THR:HG21	1:F:130:ILE:HD11	2.02	0.41
1:G:18:MET:HB2	1:G:22:SER:HB2	2.02	0.41
1:E:175:MET:HB3	1:E:179:GLU:HB2	2.02	0.41
1:F:129:ILE:HG22	1:F:131:GLY:H	1.86	0.40
1:C:7:VAL:HG11	1:C:23:ARG:HB2	2.02	0.40
1:E:138:LEU:HD12	1:E:142:GLU:HB3	2.04	0.40
1:G:132:THR:O	1:G:136:ILE:HA	2.22	0.40
1:A:52:MET:HE3	1:A:52:MET:HB3	1.95	0.40
1:A:145:THR:HG21	1:C:119:ARG:CZ	2.51	0.40
1:C:153:ILE:HD11	1:E:117:HIS:CE1	2.57	0.40
1:A:174:PHE:HB2	1:F:142:GLU:OE1	2.21	0.40
1:F:41:ALA:HA	1:F:77:ILE:HD11	2.04	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	183/203 (90%)	170 (93%)	10 (6%)	3 (2%)	9 29
1	B	188/203 (93%)	176 (94%)	11 (6%)	1 (0%)	29 59
1	C	185/203 (91%)	172 (93%)	10 (5%)	3 (2%)	9 29
1	D	183/203 (90%)	172 (94%)	11 (6%)	0	100 100
1	E	189/203 (93%)	176 (93%)	11 (6%)	2 (1%)	14 39
1	F	184/203 (91%)	171 (93%)	9 (5%)	4 (2%)	6 21
1	G	188/203 (93%)	178 (95%)	8 (4%)	2 (1%)	14 39
All	All	1300/1421 (92%)	1215 (94%)	70 (5%)	15 (1%)	13 37

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ALA
1	B	192	SER
1	F	127	GLY
1	G	127	GLY
1	A	193	ALA
1	C	132	THR
1	E	125	PRO
1	A	136	ILE
1	C	126	SER
1	C	136	ILE
1	E	129	ILE
1	F	192	SER
1	F	128	GLY
1	F	133	SER
1	G	128	GLY

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	154/167 (92%)	150 (97%)	4 (3%)	46	78
1	B	159/167 (95%)	157 (99%)	2 (1%)	69	90
1	C	156/167 (93%)	152 (97%)	4 (3%)	46	78
1	D	154/167 (92%)	151 (98%)	3 (2%)	57	84
1	E	159/167 (95%)	158 (99%)	1 (1%)	86	95
1	F	155/167 (93%)	153 (99%)	2 (1%)	69	90
1	G	159/167 (95%)	156 (98%)	3 (2%)	57	84
All	All	1096/1169 (94%)	1077 (98%)	19 (2%)	60	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ILE
1	A	136	ILE
1	A	143	ILE
1	A	195	GLU
1	B	130	ILE
1	B	136	ILE
1	C	36	ILE
1	C	122	ILE
1	C	129	ILE
1	C	132	THR
1	D	129	ILE
1	D	138	LEU
1	D	195	GLU
1	E	143	ILE
1	F	136	ILE
1	F	189	VAL
1	G	52	MET
1	G	130	ILE
1	G	132	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	47	GLN
1	E	124	GLN
1	G	95	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	187/203 (92%)	0.03	15 (8%) 12 7	28, 41, 98, 239	0
1	B	192/203 (94%)	0.02	15 (7%) 13 7	24, 37, 123, 193	0
1	C	189/203 (93%)	0.15	14 (7%) 14 8	27, 42, 138, 214	0
1	D	187/203 (92%)	-0.01	13 (6%) 16 9	24, 38, 90, 198	0
1	E	193/203 (95%)	-0.00	20 (10%) 6 3	25, 37, 124, 253	0
1	F	188/203 (92%)	-0.14	11 (5%) 22 14	23, 36, 103, 184	0
1	G	192/203 (94%)	0.04	16 (8%) 11 6	24, 37, 113, 205	0
All	All	1328/1421 (93%)	0.01	104 (7%) 13 7	23, 38, 115, 253	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	SER	13.7
1	D	133	SER	9.4
1	D	134	ALA	9.2
1	C	132	THR	9.0
1	E	202	ALA	8.9
1	B	132	THR	8.2
1	G	135	ASP	8.1
1	G	134	ALA	7.8
1	C	130	ILE	7.4
1	A	133	SER	6.6
1	A	135	ASP	6.5
1	E	134	ALA	6.1
1	G	200	SER	6.0
1	A	137	GLN	5.7
1	D	136	ILE	5.5
1	E	133	SER	5.5
1	G	193	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	203	SER	5.3
1	F	134	ALA	5.3
1	C	134	ALA	5.3
1	C	198	ASP	5.2
1	D	135	ASP	5.2
1	A	197	LYS	5.2
1	E	135	ASP	5.2
1	A	134	ALA	5.1
1	A	131	GLY	5.0
1	B	198	ASP	4.9
1	D	194	LYS	4.9
1	F	130	ILE	4.8
1	F	131	GLY	4.8
1	E	131	GLY	4.7
1	D	132	THR	4.7
1	E	132	THR	4.4
1	G	9	GLU	4.4
1	F	135	ASP	4.1
1	C	196	THR	4.1
1	B	134	ALA	4.1
1	F	133	SER	3.9
1	G	137	GLN	3.9
1	B	135	ASP	3.8
1	D	2	THR	3.7
1	B	8	VAL	3.7
1	E	196	THR	3.7
1	A	138	LEU	3.7
1	F	137	GLN	3.7
1	E	130	ILE	3.7
1	E	198	ASP	3.6
1	F	132	THR	3.7
1	D	137	GLN	3.6
1	B	131	GLY	3.6
1	C	135	ASP	3.6
1	E	199	LYS	3.6
1	G	16	ARG	3.6
1	G	132	THR	3.5
1	A	196	THR	3.5
1	C	17	ALA	3.5
1	G	133	SER	3.4
1	C	136	ILE	3.4
1	C	131	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	196	THR	3.2
1	B	126	SER	3.1
1	F	196	THR	3.1
1	B	195	GLU	3.1
1	A	17	ALA	3.1
1	B	196	THR	3.0
1	E	201	ILE	3.0
1	B	9	GLU	2.9
1	E	137	GLN	2.9
1	E	17	ALA	2.9
1	F	197	LYS	2.9
1	G	57	THR	2.8
1	E	3	LEU	2.8
1	G	138	LEU	2.8
1	A	136	ILE	2.7
1	A	3	LEU	2.7
1	B	55	ASP	2.7
1	E	138	LEU	2.7
1	A	132	THR	2.6
1	C	137	GLN	2.6
1	B	16	ARG	2.6
1	C	8	VAL	2.5
1	B	199	LYS	2.5
1	E	193	ALA	2.4
1	G	8	VAL	2.4
1	F	3	LEU	2.4
1	B	17	ALA	2.4
1	C	3	LEU	2.3
1	D	3	LEU	2.3
1	D	127	GLY	2.3
1	G	17	ALA	2.2
1	G	197	LYS	2.2
1	D	196	THR	2.2
1	B	133	SER	2.2
1	E	192	SER	2.2
1	A	193	ALA	2.1
1	E	191	SER	2.1
1	A	8	VAL	2.1
1	D	17	ALA	2.1
1	D	131	GLY	2.1
1	A	130	ILE	2.1
1	C	126	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	3	LEU	2.0
1	E	55	ASP	2.0
1	F	193	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 monosaccharides 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.