



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 07:20 AM EDT

PDB ID : 3OTV
Title : Crystal structure of the intracellular domain of Rv3910 from Mycobacterium tuberculosis
Authors : Gee, C.L.; Alber, T.
Deposited on : 2010-09-14
Resolution : 3.09 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 : 2.36
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) : 2.36

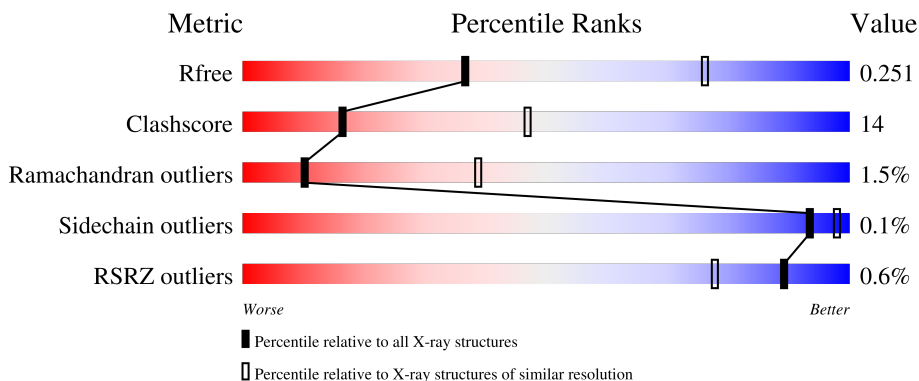
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	285	
1	B	285	
1	C	285	
1	D	285	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7513 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 PROBABLE CONSERVED TRANSMEMBRANE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	Total 1890	C 1182	N 350	O 355	S 3	63	0	0
1	B	244	Total 1815	C 1135	N 336	O 341	S 3	34	0	0
1	C	257	Total 1911	C 1193	N 353	O 362	S 3	60	0	0
1	D	248	Total 1837	C 1150	N 338	O 346	S 3	64	0	0

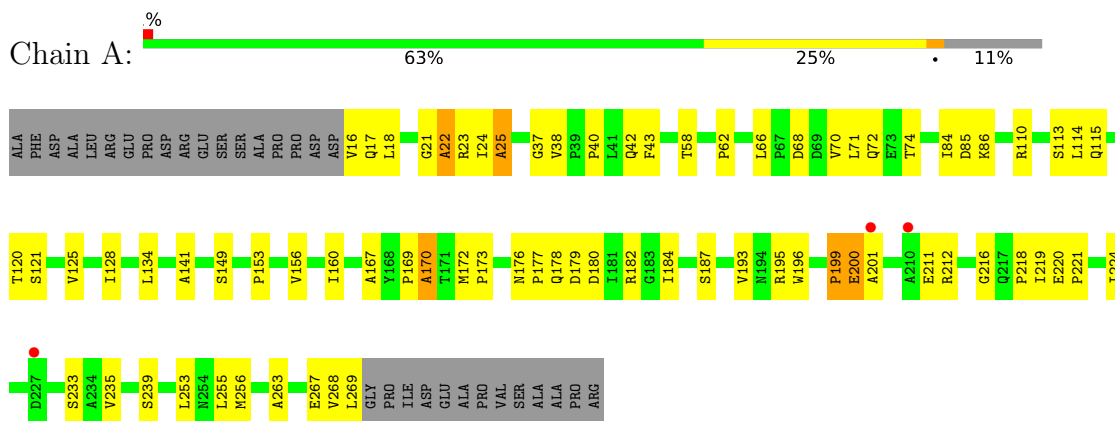
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	O 7	0	0
2	B	28	Total 28	O 28	0	0
2	C	11	Total 11	O 11	0	0
2	D	14	Total 14	O 14	0	0

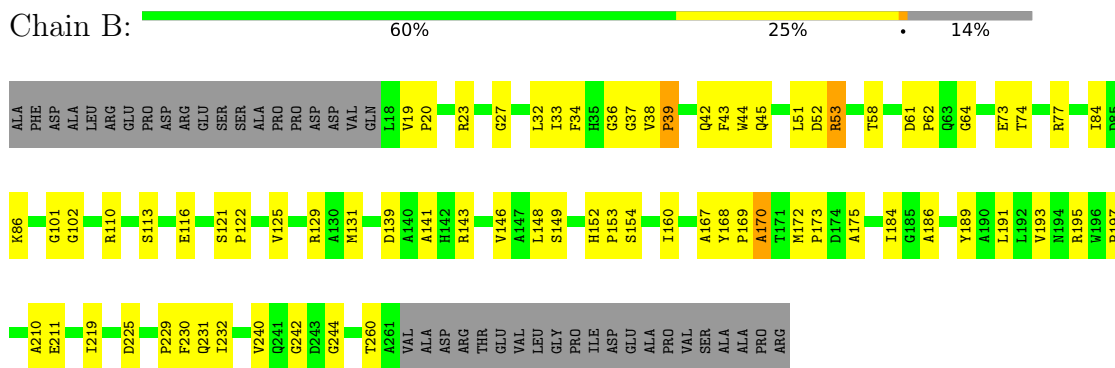
3 Residue-property plots

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.

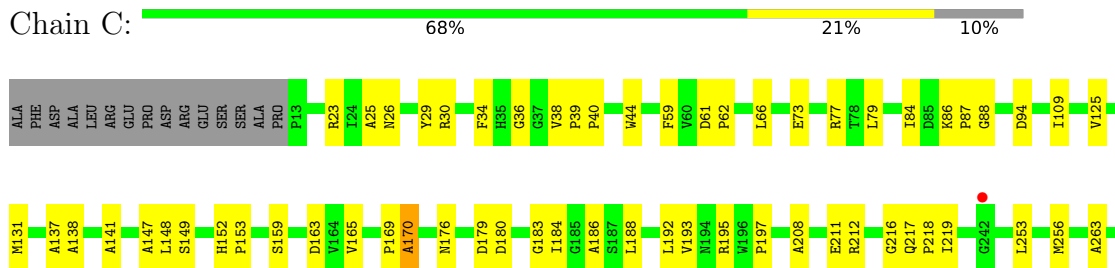
- Molecule 1: PROBABLE CONSERVED TRANSMEMBRANE PROTEIN



- Molecule 1: PROBABLE CONSERVED TRANSMEMBRANE PROTEIN



- Molecule 1: PROBABLE CONSERVED TRANSMEMBRANE PROTEIN



T266
E267
V268
L269
GLY
PRO
ILE
ASP
GLU
ALA
PRO
VAL
SER
ALA
ALA
PRO
ARG

● Molecule 1: PROBABLE CONSERVED TRANSMEMBRANE PROTEIN

Chain D: 64% 22% 13%

ALA
PHE
ASP
ALA
LEU
ARG
GLU
PRO
ASP
ARG
GLU
SER
SER
ALA
PRO
PRO
ASP
ASP
V16
A22
R23
I24
R30
L31
F34
H35
G36
G37
V38
P39
F43
T58
F59
V60
D61
P62
R77
I84
D85
K86
V89
A90
R91
E107
I128
R129
A130
M131
A137

A138
D139
V146
A147
I150
H152
P153
L166
A167
Y168
P169
A170
P173
M176
P177
I184
L188
A201
G202
V203
E211
R212
D213
Q217
P218
I219
D223
I224
D225
R226
Q231
A234
V235
A236
A237
R238
Q241
G242
D243
G244
A249
L252

M256
Q257
Q258
V262
A263
ASP
ARG
THR
GLU
GLU
VAL
LEU
GLY
PRO
ILE
ASP
GLU
ALA
PRO
VAL
SER
ALA
ALA
PRO
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.04Å 59.69Å 145.06Å 90.00° 97.21° 90.00°	Depositor
Resolution (Å)	40.81 – 3.09 40.81 – 3.09	Depositor EDS
% Data completeness (in resolution range)	87.3 (40.81-3.09) 87.4 (40.81-3.09)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.12Å)	Xtrriage
Refinement program	ELVES, PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.189 , 0.248 0.188 , 0.251	Depositor DCC
R_{free} test set	829 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtrriage
Anisotropy	0.122	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7513	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% 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](#)

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	0.47	0/1924	0.65	0/2630
1	B	0.49	0/1849	0.72	0/2527
1	C	0.47	0/1945	0.67	0/2659
1	D	0.44	0/1871	0.64	0/2559
All	All	0.47	0/7589	0.67	0/10375

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	1890	0	1912	55	0
1	B	1815	0	1833	62	0
1	C	1911	0	1922	47	0
1	D	1837	0	1853	44	0
2	A	7	0	0	0	0
2	B	28	0	0	1	0
2	C	11	0	0	0	0
2	D	14	0	0	0	0
All	All	7513	0	7520	207	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 14.

All (207) 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:A:16:VAL:HG12	1:A:17:GLN:H	1.12	1.09
1:B:131:MET:CE	1:B:184:ILE:HG23	2.08	0.84
1:A:16:VAL:HG12	1:A:17:GLN:N	1.93	0.84
1:B:113:SER:OG	1:B:116:GLU:HG3	1.77	0.83
1:C:40:PRO:HG3	1:C:66:LEU:HD11	1.63	0.81
1:A:211:GLU:HB2	1:A:219:ILE:HD12	1.62	0.79
1:C:61:ASP:HB2	1:C:66:LEU:HD12	1.64	0.79
1:D:258:GLN:O	1:D:262:VAL:HG23	1.83	0.79
1:B:73:GLU:O	1:B:77:ARG:HG3	1.84	0.76
1:A:16:VAL:CG1	1:A:17:GLN:H	1.97	0.72
1:B:58:THR:OG1	1:B:168:TYR:HB3	1.89	0.72
1:D:211:GLU:HB3	1:D:219:ILE:HD12	1.71	0.72
1:B:32:LEU:HB2	1:B:45:GLN:O	1.90	0.71
1:A:153:PRO:HG3	1:A:196:TRP:CE3	2.25	0.71
1:C:88:GLY:HA3	1:C:137:ALA:HB2	1.70	0.71
1:B:129:ARG:HE	1:B:260:THR:HG21	1.55	0.70
1:A:172:MET:HB3	1:A:173:PRO:HD2	1.72	0.69
1:A:125:VAL:HG22	1:A:263:ALA:HB1	1.75	0.69
1:A:153:PRO:HG3	1:A:196:TRP:CD2	2.29	0.68
1:C:34:PHE:CZ	1:C:36:GLY:HA2	2.28	0.68
1:D:89:VAL:HG23	1:D:137:ALA:HB1	1.74	0.68
1:D:150:ILE:HG22	1:D:150:ILE:O	1.94	0.68
1:B:113:SER:HG	1:B:116:GLU:HG3	1.59	0.66
1:D:152:HIS:ND1	1:D:153:PRO:HD2	2.11	0.64
1:A:167:ALA:O	1:A:169:PRO:HD3	1.98	0.64
1:B:23:ARG:HB3	1:B:27:GLY:HA2	1.80	0.64
1:B:131:MET:HE1	1:B:184:ILE:HG23	1.77	0.64
1:B:51:LEU:HD21	1:C:94:ASP:HA	1.81	0.63
1:D:152:HIS:CE1	1:D:153:PRO:HD2	2.34	0.63
1:B:53:ARG:HD2	2:B:298:HOH:O	1.98	0.63
1:C:38:VAL:HG23	1:C:38:VAL:O	1.98	0.63
1:A:68:ASP:O	1:A:72:GLN:HG2	2.00	0.61
1:B:110:ARG:HH12	1:B:160:ILE:HD13	1.67	0.60
1:C:34:PHE:HB2	1:C:44:TRP:CZ2	2.35	0.60
1:D:38:VAL:O	1:D:39:PRO:C	2.40	0.60
1:B:152:HIS:ND1	1:B:153:PRO:HD2	2.17	0.59
1:B:211:GLU:HB3	1:B:219:ILE:HD12	1.84	0.59
1:D:84:ILE:HD12	1:D:84:ILE:O	2.02	0.59
1:A:176:ASN:ND2	1:A:179:ASP:OD1	2.32	0.58
1:D:58:THR:HG21	1:D:170:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PHE:CE1	1:C:36:GLY:HA2	2.39	0.58
1:A:263:ALA:O	1:A:267:GLU:HB2	2.04	0.57
1:A:212:ARG:NH1	1:A:218:PRO:HG3	2.19	0.57
1:A:199:PRO:O	1:A:200:GLU:HB3	2.04	0.57
1:C:131:MET:CE	1:C:184:ILE:HG23	2.34	0.57
1:B:33:ILE:HB	1:B:45:GLN:HB3	1.86	0.57
1:B:131:MET:HE2	1:B:184:ILE:HG23	1.86	0.57
1:D:34:PHE:CZ	1:D:36:GLY:HA2	2.39	0.57
1:A:84:ILE:CD1	1:A:141:ALA:HA	2.35	0.56
1:A:58:THR:HG21	1:A:170:ALA:HB2	1.87	0.56
1:A:70:VAL:HG13	1:A:173:PRO:HG2	1.88	0.56
1:B:172:MET:HB3	1:B:173:PRO:CD	2.35	0.56
1:A:268:VAL:HG13	1:A:269:LEU:HG	1.89	0.55
1:A:40:PRO:HG3	1:A:66:LEU:HD21	1.87	0.55
1:D:16:VAL:HG11	1:D:24:ILE:HG22	1.88	0.55
1:B:84:ILE:CD1	1:B:141:ALA:HA	2.37	0.54
1:B:84:ILE:HD11	1:B:141:ALA:HA	1.89	0.54
1:B:193:VAL:O	1:B:195:ARG:HG2	2.08	0.53
1:C:183:GLY:O	1:C:186:ALA:HB3	2.08	0.53
1:B:34:PHE:HB2	1:B:44:TRP:CH2	2.43	0.53
1:A:24:ILE:O	1:A:25:ALA:HB3	2.08	0.53
1:A:211:GLU:CB	1:A:219:ILE:HD12	2.36	0.53
1:C:73:GLU:O	1:C:77:ARG:HG3	2.09	0.53
1:D:59:PHE:HB3	1:D:62:PRO:HG3	1.90	0.53
1:A:268:VAL:HG13	1:A:269:LEU:N	2.24	0.52
1:B:58:THR:HG1	1:B:168:TYR:HB3	1.75	0.52
1:D:61:ASP:N	1:D:62:PRO:HD3	2.24	0.52
1:D:152:HIS:CG	1:D:153:PRO:HD2	2.44	0.52
1:B:101:GLY:O	1:B:102:GLY:C	2.49	0.51
1:A:169:PRO:O	1:A:170:ALA:HB2	2.11	0.51
1:A:172:MET:HB3	1:A:173:PRO:CD	2.40	0.51
1:A:38:VAL:HG13	1:A:201:ALA:O	2.10	0.51
1:B:186:ALA:HA	1:B:197:PRO:HG3	1.93	0.51
1:C:147:ALA:HB1	1:C:180:ASP:OD2	2.10	0.50
1:B:61:ASP:OD2	1:B:64:GLY:N	2.45	0.50
1:A:184:ILE:O	1:A:187:SER:HB2	2.12	0.50
1:C:40:PRO:CG	1:C:66:LEU:HD11	2.37	0.50
1:D:131:MET:CE	1:D:184:ILE:HG23	2.42	0.50
1:A:120:THR:O	1:A:121:SER:C	2.50	0.49
1:B:51:LEU:O	1:B:52:ASP:C	2.49	0.49
1:B:197:PRO:HB2	1:B:240:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:HB2	1:A:115:GLN:OE1	2.12	0.49
1:D:152:HIS:CG	1:D:153:PRO:CD	2.95	0.49
1:C:211:GLU:HB2	1:C:219:ILE:HD12	1.95	0.49
1:C:169:PRO:O	1:C:170:ALA:HB2	2.13	0.48
1:D:176:ASN:OD1	1:D:177:PRO:HD2	2.13	0.48
1:B:129:ARG:HH21	1:B:260:THR:HG22	1.77	0.48
1:A:42:GLN:NE2	1:A:62:PRO:HG2	2.28	0.48
1:B:113:SER:OG	1:B:116:GLU:CG	2.58	0.48
1:C:125:VAL:HG13	1:C:263:ALA:HB3	1.95	0.48
1:D:84:ILE:HD13	1:D:86:LYS:HG3	1.96	0.48
1:D:38:VAL:HG22	1:D:201:ALA:O	2.13	0.48
1:C:84:ILE:HG23	1:C:86:LYS:HG3	1.95	0.48
1:C:138:ALA:HA	1:C:148:LEU:CD1	2.42	0.48
1:C:138:ALA:HA	1:C:148:LEU:HD11	1.96	0.48
1:B:125:VAL:O	1:B:129:ARG:HB2	2.14	0.48
1:C:61:ASP:HB2	1:C:66:LEU:CD1	2.41	0.48
1:B:168:TYR:CD1	1:B:168:TYR:N	2.82	0.47
1:D:43:PHE:HB3	1:D:168:TYR:CE2	2.50	0.47
1:D:242:GLY:C	1:D:244:GLY:N	2.67	0.47
1:B:148:LEU:O	1:B:149:SER:HB3	2.14	0.47
1:B:42:GLN:NE2	1:B:62:PRO:HG2	2.30	0.47
1:B:141:ALA:HB1	1:B:146:VAL:O	2.15	0.47
1:C:23:ARG:HA	1:C:29:TYR:O	2.15	0.47
1:C:212:ARG:HD2	1:C:216:GLY:O	2.15	0.47
1:B:149:SER:HB2	1:B:175:ALA:HB2	1.96	0.47
1:B:38:VAL:O	1:B:39:PRO:C	2.53	0.47
1:A:21:GLY:O	1:A:23:ARG:HD2	2.15	0.47
1:C:193:VAL:O	1:C:193:VAL:CG1	2.63	0.47
1:D:128:ILE:HG23	1:D:129:ARG:N	2.30	0.47
1:D:231:GLN:O	1:D:235:VAL:HG23	2.15	0.47
1:C:266:THR:HG22	1:C:266:THR:O	2.16	0.46
1:D:241:GLN:O	1:D:241:GLN:HG3	2.16	0.46
1:A:235:VAL:HG22	1:A:255:LEU:HB3	1.96	0.46
1:C:34:PHE:CZ	1:C:36:GLY:CA	2.96	0.46
1:C:23:ARG:HG2	1:C:30:ARG:HG3	1.98	0.46
1:A:235:VAL:O	1:A:239:SER:HB3	2.15	0.46
1:D:223:ASP:HA	1:D:226:ARG:HH12	1.81	0.46
1:D:234:ALA:O	1:D:238:ARG:HG3	2.15	0.46
1:A:18:LEU:HD12	1:A:42:GLN:OE1	2.16	0.46
1:A:211:GLU:HB2	1:A:219:ILE:CD1	2.40	0.46
1:B:242:GLY:C	1:B:244:GLY:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PHE:HB2	1:C:44:TRP:CH2	2.51	0.46
1:D:24:ILE:HD12	1:D:24:ILE:C	2.35	0.46
1:A:221:PRO:HD2	1:A:233:SER:OG	2.16	0.46
1:D:242:GLY:O	1:D:244:GLY:N	2.49	0.46
1:C:188:LEU:O	1:C:192:LEU:HG	2.15	0.45
1:B:189:TYR:OH	1:B:210:ALA:HB1	2.16	0.45
1:C:163:ASP:O	1:C:165:VAL:HG23	2.15	0.45
1:A:253:LEU:O	1:A:256:MET:HB2	2.17	0.45
1:A:58:THR:HG21	1:A:170:ALA:CB	2.46	0.45
1:A:128:ILE:HD11	1:A:256:MET:HA	1.99	0.45
1:B:74:THR:OG1	1:B:172:MET:HA	2.17	0.45
1:B:37:GLY:HA2	1:B:43:PHE:CE1	2.51	0.45
1:C:25:ALA:O	1:C:26:ASN:HB2	2.16	0.45
1:A:212:ARG:HD2	1:A:216:GLY:O	2.17	0.44
1:A:153:PRO:HD3	1:A:196:TRP:CE2	2.53	0.44
1:C:38:VAL:O	1:C:39:PRO:C	2.56	0.44
1:C:253:LEU:O	1:C:256:MET:HB2	2.17	0.44
1:A:193:VAL:O	1:A:195:ARG:HG2	2.17	0.44
1:B:152:HIS:CE1	1:B:154:SER:HB2	2.52	0.44
1:B:230:PHE:O	1:B:231:GLN:C	2.56	0.44
1:A:177:PRO:O	1:A:180:ASP:HB2	2.18	0.44
1:C:266:THR:O	1:C:267:GLU:C	2.55	0.44
1:D:188:LEU:HD23	1:D:236:ALA:HB2	2.00	0.44
1:A:37:GLY:HA2	1:A:43:PHE:CE1	2.53	0.43
1:D:58:THR:HG21	1:D:170:ALA:CB	2.46	0.43
1:D:77:ARG:HD3	1:D:173:PRO:HA	1.99	0.43
1:D:219:ILE:HG22	1:D:224:ILE:HG13	2.00	0.43
1:B:34:PHE:CZ	1:B:36:GLY:HA2	2.54	0.43
1:B:58:THR:HG21	1:B:170:ALA:HB2	1.99	0.43
1:C:266:THR:O	1:C:266:THR:CG2	2.66	0.43
1:D:252:LEU:O	1:D:256:MET:HG3	2.17	0.43
1:B:129:ARG:HE	1:B:260:THR:CG2	2.26	0.43
1:B:152:HIS:ND1	1:B:154:SER:HB2	2.33	0.43
1:C:84:ILE:CG2	1:C:86:LYS:HG3	2.49	0.43
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.88	0.43
1:B:129:ARG:HH21	1:B:260:THR:CG2	2.32	0.43
1:C:148:LEU:O	1:C:149:SER:HB3	2.18	0.43
1:B:58:THR:HG21	1:B:170:ALA:CB	2.49	0.43
1:B:152:HIS:CE1	1:B:153:PRO:HD2	2.54	0.43
1:B:139:ASP:O	1:B:143:ARG:HG3	2.17	0.43
1:B:225:ASP:OD2	1:B:225:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:VAL:HG22	1:D:147:ALA:N	2.34	0.43
1:A:211:GLU:O	1:A:219:ILE:HG13	2.19	0.43
1:D:43:PHE:HB3	1:D:168:TYR:CD2	2.54	0.43
1:B:51:LEU:CD1	1:B:51:LEU:N	2.81	0.42
1:D:184:ILE:O	1:D:184:ILE:HG22	2.20	0.42
1:A:21:GLY:O	1:A:22:ALA:C	2.58	0.42
1:C:79:LEU:HA	1:C:79:LEU:HD23	1.77	0.42
1:A:125:VAL:CG2	1:A:263:ALA:HB1	2.47	0.42
1:A:85:ASP:C	1:A:86:LYS:HG2	2.40	0.42
1:D:22:ALA:HB3	1:D:31:LEU:HD12	2.02	0.42
1:D:91:ARG:H	1:D:107:GLU:HG2	1.84	0.42
1:A:220:GLU:O	1:A:224:ILE:HG13	2.19	0.42
1:B:167:ALA:O	1:B:169:PRO:HD3	2.20	0.42
1:C:38:VAL:O	1:C:38:VAL:CG2	2.68	0.42
1:C:86:LYS:HA	1:C:87:PRO:HD3	1.91	0.42
1:D:84:ILE:HD12	1:D:84:ILE:C	2.40	0.42
1:A:178:GLN:O	1:A:182:ARG:HG3	2.19	0.42
1:B:172:MET:HB3	1:B:173:PRO:HD2	2.02	0.42
1:B:121:SER:HA	1:B:122:PRO:HD2	1.85	0.42
1:C:59:PHE:HB3	1:C:62:PRO:HG3	2.02	0.42
1:C:176:ASN:ND2	1:C:179:ASP:OD1	2.52	0.42
1:D:23:ARG:HD2	1:D:30:ARG:NH2	2.34	0.42
1:C:152:HIS:CG	1:C:153:PRO:HD2	2.54	0.41
1:A:263:ALA:O	1:A:267:GLU:N	2.52	0.41
1:A:114:LEU:HB2	1:A:156:VAL:HG23	2.02	0.41
1:B:186:ALA:HA	1:B:197:PRO:CG	2.50	0.41
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.87	0.41
1:C:217:GLN:HA	1:C:218:PRO:HD3	1.91	0.41
1:A:71:LEU:O	1:A:74:THR:HB	2.21	0.41
1:D:257:GLN:HE21	1:D:257:GLN:HB2	1.55	0.41
1:A:84:ILE:HD12	1:A:141:ALA:HA	2.02	0.41
1:B:110:ARG:NH1	1:B:160:ILE:HD13	2.35	0.41
1:B:229:PRO:HB2	1:B:232:ILE:HG13	2.03	0.41
1:C:109:ILE:CG2	1:C:159:SER:HB3	2.50	0.41
1:C:186:ALA:HA	1:C:197:PRO:HG2	2.02	0.41
1:D:213:ASP:OD2	1:D:217:GLN:HB2	2.21	0.41
1:B:19:VAL:HB	1:B:20:PRO:HD2	2.03	0.41
1:D:167:ALA:O	1:D:169:PRO:HD3	2.21	0.41
1:B:84:ILE:CG2	1:B:86:LYS:HG3	2.51	0.40
1:D:139:ASP:HA	1:D:249:ALA:HB3	2.03	0.40
1:A:110:ARG:NH1	1:A:160:ILE:HD13	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:HH11	1:B:53:ARG:CG	2.34	0.40
1:C:195:ARG:CD	1:C:208:ALA:HB3	2.51	0.40
1:C:138:ALA:O	1:C:141:ALA:HB3	2.21	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	252/285 (88%)	224 (89%)	22 (9%)	6 (2%)	6 27
1	B	242/285 (85%)	222 (92%)	18 (7%)	2 (1%)	19 54
1	C	255/285 (90%)	240 (94%)	14 (6%)	1 (0%)	34 69
1	D	246/285 (86%)	224 (91%)	16 (6%)	6 (2%)	6 27
All	All	995/1140 (87%)	910 (92%)	70 (7%)	15 (2%)	10 39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ALA
1	C	170	ALA
1	B	170	ALA
1	D	170	ALA
1	A	200	GLU
1	D	243	ASP
1	A	22	ALA
1	A	25	ALA
1	B	39	PRO
1	D	107	GLU
1	D	166	LEU
1	A	149	SER

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Mol	Chain	Res	Type
1	D	203	VAL
1	A	199	PRO
1	D	39	PRO

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	196/221 (89%)	196 (100%)	0	100	100
1	B	188/221 (85%)	187 (100%)	1 (0%)	88	94
1	C	198/221 (90%)	198 (100%)	0	100	100
1	D	190/221 (86%)	190 (100%)	0	100	100
All	All	772/884 (87%)	771 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	C	257	GLN
1	D	132	GLN
1	D	257	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	254/285 (89%)	-0.20	3 (1%) 79 61	34, 62, 96, 115	13 (5%)
1	B	244/285 (85%)	-0.40	0 100 100	35, 51, 74, 105	8 (3%)
1	C	257/285 (90%)	-0.25	1 (0%) 92 84	35, 61, 92, 101	13 (5%)
1	D	248/285 (87%)	-0.35	2 (0%) 86 72	36, 61, 85, 96	13 (5%)
All	All	1003/1140 (87%)	-0.30	6 (0%) 89 78	34, 58, 90, 115	47 (4%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	ASP	3.1
1	C	242	GLY	2.7
1	D	262	VAL	2.4
1	A	201	ALA	2.1
1	D	202	GLY	2.1
1	A	210	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.