Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 08:35 am BST

PDB ID	:	5FQ3
Title	:	Crystal structure of the lipoprotein BT2262 from Bacteroides thetaiotaomicron
Authors	:	Glenwright, A.J.; Pothula, K.R.; Chorev, D.S.; Basle, A.; Robinson, C.V.; Kleinekathoefer, U.; Bolam, D.N.; van den Berg, B.
Deposited on	:	2015-12-04
Resolution	:	3.10 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

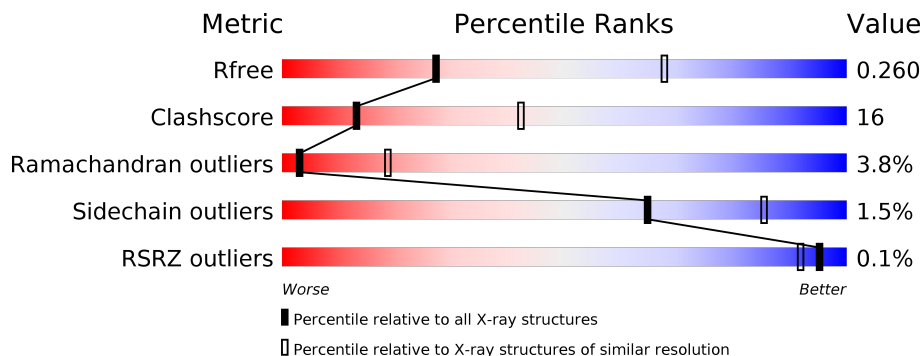|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	Percentile Ranks	Value
Rfree		0.260
Clashscore		16
Ramachandran outliers		3.8%
Sidechain outliers		1.5%
RSRZ outliers		0.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 on 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	213	69% 21% • 7%
1	B	213	64% 27% • 7%
1	C	213	62% 29% • 7%
1	D	213	57% 32% • 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6180 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 BT_2262.

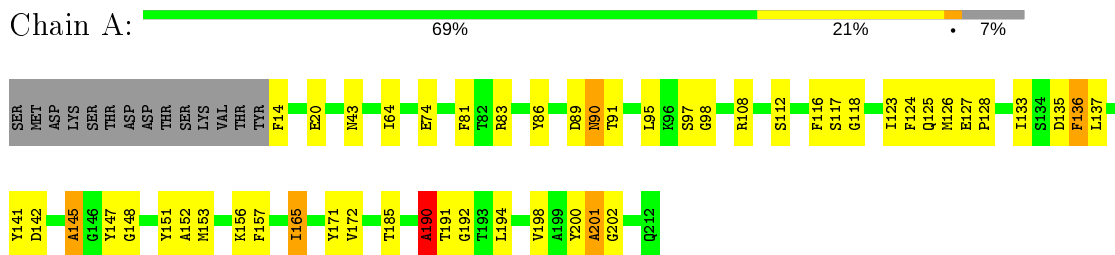| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total 1545	C 993	N 238	O 309	S 5	0	0	0
1	B	199	Total 1545	C 993	N 238	O 309	S 5	0	0	0
1	C	199	Total 1545	C 993	N 238	O 309	S 5	0	0	0
1	D	199	Total 1545	C 993	N 238	O 309	S 5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

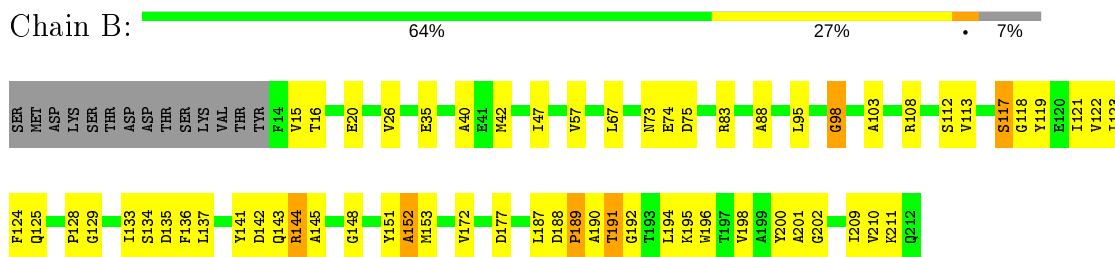| Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q8A5H7
A	1	MET	-	expression tag	UNP Q8A5H7
B	0	SER	-	expression tag	UNP Q8A5H7
B	1	MET	-	expression tag	UNP Q8A5H7
C	0	SER	-	expression tag	UNP Q8A5H7
C	1	MET	-	expression tag	UNP Q8A5H7
D	0	SER	-	expression tag	UNP Q8A5H7
D	1	MET	-	expression tag	UNP Q8A5H7

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.
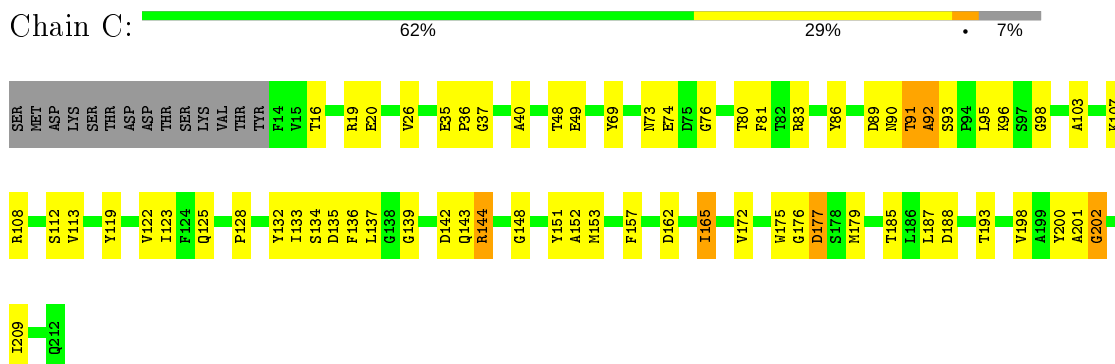
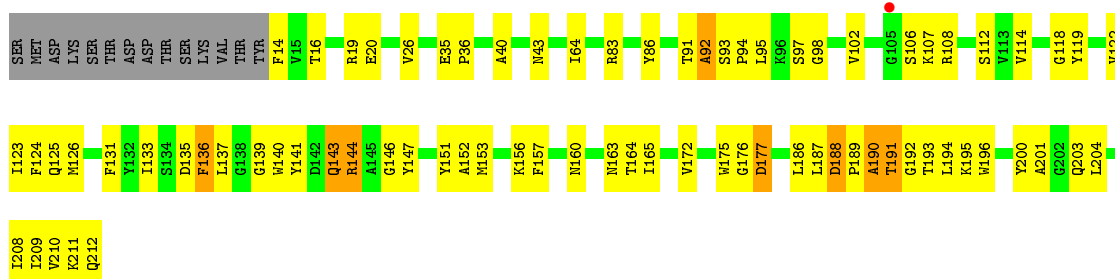- Molecule 1: BT_2262

Chain A:

- Molecule 1: BT_2262

Chain B:

- Molecule 1: BT_2262

Chain C:

- Molecule 1: BT_2262

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.32Å 167.32Å 100.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 3.10 48.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.75-3.10) 95.9 (48.75-3.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.73 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.199 , 0.260 0.199 , 0.260	Depositor DCC
R_{free} test set	1999 reflections (7.57%)	wwPDB-VP
Wilson B-factor (Å^2)	80.6	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.4	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6180	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.52	0/1583	0.78	1/2156 (0.0%)
1	B	0.52	0/1583	0.78	0/2156
1	C	0.48	0/1583	0.75	1/2156 (0.0%)
1	D	0.45	0/1583	0.73	0/2156
All	All	0.49	0/6332	0.76	2/8624 (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	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	165	ILE	CG1-CB-CG2	-5.22	99.92	111.40
1	A	165	ILE	CG1-CB-CG2	-5.11	100.17	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	PHE	Peptide
1	A	190	ALA	Peptide
1	B	129	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	107	LYS	Peptide
1	D	190	ALA	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	1545	0	1470	36	0
1	B	1545	0	1470	49	0
1	C	1545	0	1470	47	0
1	D	1545	0	1470	69	0
All	All	6180	0	5880	196	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 16.

All (196) 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:20:GLU:O	1:D:83:ARG:NH2	2.12	0.83
1:D:188:ASP:HB2	1:D:193:THR:HG22	1.60	0.82
1:B:153:MET:HE1	1:B:198:VAL:HG21	1.64	0.79
1:A:153:MET:HE1	1:A:198:VAL:HG21	1.64	0.77
1:D:137:LEU:HD13	1:D:153:MET:HG3	1.66	0.77
1:D:194:LEU:HD23	1:D:196:TRP:HZ3	1.51	0.76
1:D:123:ILE:HG22	1:D:133:ILE:HG13	1.67	0.76
1:B:20:GLU:O	1:B:83:ARG:NH2	2.19	0.75
1:C:123:ILE:HG12	1:C:133:ILE:HG22	1.68	0.74
1:B:75:ASP:OD2	1:D:19:ARG:NH2	2.19	0.74
1:D:194:LEU:HD23	1:D:196:TRP:CZ3	2.24	0.73
1:D:136:PHE:HB2	1:D:153:MET:HB2	1.72	0.72
1:A:108:ARG:HH21	1:A:112:SER:HB3	1.55	0.71
1:B:187:LEU:HG	1:B:189:PRO:HA	1.72	0.70
1:A:20:GLU:O	1:A:83:ARG:NH2	2.24	0.69
1:A:89:ASP:O	1:A:91:THR:N	2.26	0.69
1:B:137:LEU:HD13	1:B:153:MET:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ASN:HD21	1:D:189:PRO:HD3	1.59	0.68
1:A:123:ILE:HG12	1:A:133:ILE:HG22	1.74	0.68
1:D:126:MET:HE1	1:D:156:LYS:HE3	1.76	0.68
1:D:135:ASP:CG	1:D:152:ALA:HB1	2.14	0.68
1:C:20:GLU:O	1:C:83:ARG:NH2	2.28	0.67
1:B:188:ASP:HB3	1:B:189:PRO:O	1.95	0.67
1:B:191:THR:HB	1:B:192:GLY:HA2	1.77	0.67
1:B:135:ASP:CG	1:B:152:ALA:HB1	2.15	0.67
1:C:153:MET:HE3	1:C:198:VAL:HG21	1.76	0.66
1:B:151:TYR:O	1:B:152:ALA:HB3	1.95	0.66
1:D:108:ARG:HH21	1:D:112:SER:HB2	1.61	0.65
1:D:144:ARG:O	1:D:146:GLY:N	2.28	0.64
1:B:73:ASN:OD1	1:B:74:GLU:N	2.31	0.63
1:A:151:TYR:O	1:A:152:ALA:HB3	1.99	0.62
1:B:133:ILE:HG21	1:B:136:PHE:CE1	2.35	0.62
1:B:122:VAL:HG12	1:B:134:SER:HB3	1.81	0.62
1:A:157:PHE:CD1	1:A:165:ILE:HG13	2.35	0.61
1:D:95:LEU:HB3	1:D:131:PHE:CZ	2.35	0.61
1:B:190:ALA:HA	1:B:192:GLY:CA	2.30	0.61
1:A:97:SER:HB3	1:A:124:PHE:HA	1.84	0.60
1:B:117:SER:OG	1:B:118:GLY:N	2.31	0.60
1:D:114:VAL:HG21	1:D:140:TRP:CH2	2.36	0.60
1:D:137:LEU:HD23	1:D:141:TYR:HD2	1.66	0.60
1:A:117:SER:OG	1:A:118:GLY:N	2.33	0.60
1:C:188:ASP:HB3	1:C:193:THR:HG22	1.84	0.60
1:C:135:ASP:CG	1:C:152:ALA:HB1	2.21	0.59
1:C:200:TYR:O	1:C:202:GLY:N	2.35	0.59
1:C:142:ASP:HB3	1:C:148:GLY:O	2.03	0.59
1:B:142:ASP:HB3	1:B:148:GLY:C	2.23	0.59
1:A:135:ASP:CG	1:A:152:ALA:HB1	2.24	0.58
1:B:112:SER:OG	1:B:113:VAL:N	2.35	0.58
1:A:133:ILE:O	1:A:133:ILE:HD12	2.02	0.58
1:D:188:ASP:OD1	1:D:190:ALA:HB3	2.02	0.58
1:A:142:ASP:HB3	1:A:148:GLY:O	2.04	0.58
1:D:125:GLN:HB3	1:D:131:PHE:CE2	2.39	0.58
1:A:136:PHE:HB2	1:A:153:MET:HB2	1.86	0.57
1:D:151:TYR:O	1:D:152:ALA:HB3	2.03	0.57
1:D:139:GLY:HA3	1:D:143:GLN:HG3	1.86	0.57
1:C:125:GLN:NE2	1:C:128:PRO:O	2.37	0.56
1:C:135:ASP:OD2	1:C:139:GLY:N	2.35	0.56
1:B:125:GLN:NE2	1:B:128:PRO:O	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:C	1:A:192:GLY:H	2.09	0.56
1:B:190:ALA:HA	1:B:192:GLY:HA2	1.87	0.55
1:C:136:PHE:HB2	1:C:153:MET:HB2	1.87	0.55
1:C:48:THR:HG22	1:D:176:GLY:HA2	1.89	0.54
1:D:93:SER:C	1:D:95:LEU:H	2.10	0.54
1:A:190:ALA:O	1:A:191:THR:OG1	2.23	0.54
1:D:107:LYS:HB2	1:D:114:VAL:O	2.07	0.54
1:A:165:ILE:HG22	1:A:185:THR:CB	2.38	0.53
1:D:102:VAL:HB	1:D:118:GLY:HA2	1.90	0.53
1:C:153:MET:HG2	1:C:172:VAL:CG2	2.39	0.53
1:D:119:TYR:OH	1:D:144:ARG:HG2	2.09	0.53
1:C:133:ILE:O	1:C:133:ILE:HD12	2.08	0.53
1:D:106:SER:OG	1:D:209:ILE:N	2.36	0.52
1:C:151:TYR:O	1:C:152:ALA:HB3	2.09	0.52
1:A:64:ILE:HG12	1:A:86:TYR:CD2	2.45	0.52
1:C:89:ASP:O	1:C:91:THR:N	2.42	0.52
1:A:141:TYR:O	1:A:147:TYR:HB2	2.10	0.52
1:A:137:LEU:HD22	1:A:153:MET:HG3	1.92	0.52
1:B:136:PHE:HB2	1:B:153:MET:HB2	1.90	0.52
1:C:112:SER:OG	1:C:113:VAL:N	2.42	0.52
1:D:153:MET:HG2	1:D:172:VAL:HG22	1.91	0.52
1:D:192:GLY:O	1:D:211:LYS:HG3	2.09	0.52
1:A:153:MET:HG2	1:A:172:VAL:HG22	1.90	0.52
1:A:200:TYR:CG	1:A:201:ALA:N	2.75	0.52
1:C:69:TYR:O	1:C:80:THR:HA	2.09	0.52
1:D:93:SER:O	1:D:95:LEU:N	2.43	0.52
1:C:123:ILE:HA	1:C:132:TYR:O	2.10	0.52
1:C:35:GLU:HG3	1:C:37:GLY:H	1.75	0.51
1:C:153:MET:SD	1:C:179:MET:HB3	2.50	0.51
1:D:211:LYS:HG2	1:D:212:GLN:H	1.76	0.51
1:A:165:ILE:HG22	1:A:185:THR:HB	1.93	0.51
1:C:137:LEU:HD13	1:C:153:MET:HE2	1.91	0.51
1:B:108:ARG:NH2	1:B:112:SER:HB3	2.26	0.51
1:C:119:TYR:OH	1:C:144:ARG:HG3	2.11	0.50
1:D:211:LYS:HG2	1:D:212:GLN:N	2.26	0.50
1:B:122:VAL:CG1	1:B:134:SER:HB3	2.41	0.49
1:B:153:MET:HG2	1:B:172:VAL:HG22	1.93	0.49
1:C:49:GLU:HG2	1:D:175:TRP:HA	1.94	0.49
1:D:135:ASP:OD2	1:D:139:GLY:N	2.43	0.49
1:D:194:LEU:O	1:D:209:ILE:HA	2.13	0.49
1:D:97:SER:HB3	1:D:124:PHE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:MET:HB2	1:B:47:ILE:HD13	1.95	0.49
1:D:35:GLU:OE2	1:D:36:PRO:HD2	2.13	0.49
1:B:121:ILE:HD11	1:B:210:VAL:HG11	1.94	0.48
1:B:15:VAL:CG2	1:B:73:ASN:HD22	2.27	0.48
1:C:122:VAL:HG12	1:C:134:SER:HB3	1.94	0.48
1:D:141:TYR:O	1:D:147:TYR:HB2	2.13	0.48
1:B:26:VAL:HG21	1:B:98:GLY:HA3	1.95	0.48
1:C:176:GLY:CA	1:C:177:ASP:HB2	2.43	0.48
1:D:188:ASP:HB3	1:D:189:PRO:CA	2.43	0.48
1:A:74:GLU:OE1	1:A:74:GLU:N	2.46	0.48
1:D:14:PHE:HB2	1:D:43:ASN:OD1	2.13	0.48
1:D:137:LEU:HD23	1:D:141:TYR:CD2	2.46	0.48
1:D:98:GLY:O	1:D:122:VAL:HG23	2.13	0.48
1:B:141:TYR:O	1:B:145:ALA:HB3	2.14	0.48
1:B:16:THR:O	1:B:40:ALA:HA	2.13	0.48
1:D:153:MET:HG2	1:D:172:VAL:CG2	2.44	0.48
1:D:26:VAL:HG22	1:D:86:TYR:HB2	1.94	0.48
1:B:133:ILE:HG21	1:B:136:PHE:CD1	2.49	0.47
1:B:200:TYR:O	1:B:202:GLY:N	2.47	0.47
1:D:187:LEU:HD12	1:D:193:THR:O	2.14	0.47
1:D:137:LEU:CD2	1:D:141:TYR:HD2	2.27	0.47
1:C:137:LEU:HD13	1:C:153:MET:CE	2.44	0.47
1:B:142:ASP:HB3	1:B:148:GLY:O	2.14	0.46
1:D:125:GLN:HA	1:D:131:PHE:HA	1.97	0.46
1:C:73:ASN:OD1	1:C:74:GLU:N	2.45	0.46
1:D:188:ASP:HB3	1:D:189:PRO:HA	1.97	0.46
1:A:165:ILE:HG21	1:A:165:ILE:HD13	1.61	0.46
1:C:93:SER:O	1:C:96:LYS:NZ	2.48	0.46
1:C:157:PHE:CE1	1:C:165:ILE:HD11	2.51	0.46
1:C:16:THR:O	1:C:40:ALA:HA	2.16	0.46
1:D:102:VAL:HA	1:D:210:VAL:HG12	1.98	0.46
1:D:188:ASP:HB2	1:D:193:THR:CG2	2.38	0.46
1:C:36:PRO:HG2	1:C:83:ARG:CZ	2.46	0.45
1:A:14:PHE:HB3	1:A:43:ASN:OD1	2.15	0.45
1:A:153:MET:CE	1:A:198:VAL:HG21	2.40	0.45
1:B:98:GLY:HA2	1:B:123:ILE:O	2.15	0.45
1:D:16:THR:O	1:D:40:ALA:HA	2.16	0.45
1:D:176:GLY:CA	1:D:177:ASP:HB2	2.47	0.45
1:D:137:LEU:HD13	1:D:153:MET:CG	2.42	0.45
1:C:137:LEU:HA	1:C:137:LEU:HD12	1.70	0.44
1:D:93:SER:C	1:D:95:LEU:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PRO:O	1:B:192:GLY:HA2	2.17	0.44
1:A:157:PHE:CD2	1:A:165:ILE:HD11	2.53	0.44
1:C:187:LEU:HD12	1:C:188:ASP:H	1.82	0.44
1:A:194:LEU:HA	1:A:194:LEU:HD12	1.84	0.44
1:B:57:VAL:CG2	1:B:67:LEU:HD11	2.47	0.44
1:C:103:ALA:HB3	1:C:209:ILE:HB	2.00	0.44
1:D:157:PHE:CD1	1:D:165:ILE:HD12	2.53	0.44
1:B:194:LEU:HG	1:B:196:TRP:CZ3	2.53	0.43
1:C:19:ARG:HB2	1:C:81:PHE:CE1	2.53	0.43
1:A:125:GLN:NE2	1:A:128:PRO:O	2.44	0.43
1:B:119:TYR:CZ	1:B:144:ARG:HB2	2.52	0.43
1:B:188:ASP:HB3	1:B:189:PRO:C	2.38	0.43
1:B:88:ALA:HB2	1:B:124:PHE:HB2	1.99	0.43
1:A:108:ARG:NH2	1:A:112:SER:HB3	2.28	0.43
1:A:141:TYR:O	1:A:145:ALA:HB3	2.18	0.43
1:B:151:TYR:N	1:B:151:TYR:CD1	2.86	0.43
1:C:108:ARG:O	1:C:113:VAL:HA	2.19	0.43
1:A:81:PHE:HA	1:C:76:GLY:O	2.19	0.43
1:D:160:ASN:ND2	1:D:164:THR:OG1	2.45	0.43
1:D:97:SER:CB	1:D:124:PHE:HA	2.48	0.43
1:C:35:GLU:OE2	1:C:83:ARG:NH1	2.52	0.43
1:C:89:ASP:OD2	1:C:91:THR:OG1	2.36	0.43
1:D:192:GLY:O	1:D:193:THR:HB	2.17	0.43
1:B:122:VAL:HG12	1:B:134:SER:CB	2.49	0.42
1:B:191:THR:HB	1:B:192:GLY:CA	2.46	0.42
1:D:191:THR:HB	1:D:192:GLY:HA3	2.00	0.42
1:D:200:TYR:CG	1:D:200:TYR:O	2.72	0.42
1:A:126:MET:HE1	1:A:156:LYS:HD3	2.02	0.42
1:D:91:THR:HG23	1:D:92:ALA:O	2.19	0.42
1:B:194:LEU:HG	1:B:196:TRP:HZ3	1.84	0.42
1:B:15:VAL:HG23	1:B:73:ASN:HD22	1.85	0.42
1:A:171:TYR:CE1	1:B:35:GLU:HG2	2.54	0.42
1:B:153:MET:HG2	1:B:172:VAL:CG2	2.49	0.42
1:B:153:MET:CE	1:B:198:VAL:HG21	2.44	0.42
1:C:91:THR:HB	1:C:92:ALA:H	1.67	0.42
1:D:151:TYR:O	1:D:152:ALA:CB	2.68	0.42
1:D:165:ILE:HD13	1:D:165:ILE:HA	1.73	0.42
1:C:176:GLY:HA3	1:C:177:ASP:HB2	2.02	0.42
1:C:175:TRP:C	1:C:177:ASP:HB2	2.41	0.41
1:B:194:LEU:HD12	1:B:195:LYS:N	2.35	0.41
1:C:133:ILE:HG12	1:C:136:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ILE:HG21	1:D:123:ILE:HD13	1.84	0.41
1:D:163:ASN:ND2	1:D:189:PRO:HD3	2.32	0.41
1:D:195:LYS:HA	1:D:208:ILE:O	2.21	0.41
1:B:192:GLY:O	1:B:211:LYS:HG3	2.21	0.41
1:C:26:VAL:HG22	1:C:86:TYR:HB2	2.02	0.41
1:B:103:ALA:HB3	1:B:209:ILE:HB	2.02	0.41
1:D:64:ILE:HG12	1:D:86:TYR:CD1	2.56	0.41
1:A:127:GLU:HB2	1:A:128:PRO:HD2	2.02	0.40
1:A:153:MET:HG2	1:A:172:VAL:CG2	2.51	0.40
1:D:147:TYR:HB3	1:D:151:TYR:CD1	2.56	0.40
1:D:188:ASP:HB3	1:D:190:ALA:N	2.36	0.40
1:D:203:GLN:O	1:D:204:LEU:HG	2.21	0.40
1:C:122:VAL:CG1	1:C:134:SER:HB3	2.51	0.40
1:C:35:GLU:HG3	1:C:37:GLY:N	2.36	0.40
1:C:165:ILE:HG22	1:C:185:THR:HG21	2.02	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	197/213 (92%)	171 (87%)	20 (10%)	6 (3%)	4	23
1	B	197/213 (92%)	177 (90%)	12 (6%)	8 (4%)	3	16
1	C	197/213 (92%)	169 (86%)	19 (10%)	9 (5%)	2	15
1	D	197/213 (92%)	166 (84%)	24 (12%)	7 (4%)	3	20
All	All	788/852 (92%)	683 (87%)	75 (10%)	30 (4%)	3	19

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	145	ALA
1	A	190	ALA
1	C	90	ASN
1	C	91	THR
1	C	201	ALA
1	A	201	ALA
1	A	202	GLY
1	B	189	PRO
1	B	191	THR
1	B	201	ALA
1	D	144	ARG
1	C	177	ASP
1	D	92	ALA
1	D	191	THR
1	A	98	GLY
1	B	98	GLY
1	B	143	GLN
1	B	177	ASP
1	C	143	GLN
1	C	144	ARG
1	D	143	GLN
1	D	177	ASP
1	B	152	ALA
1	C	92	ALA
1	D	94	PRO
1	D	201	ALA
1	B	117	SER
1	C	202	GLY
1	C	98	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	163/178 (92%)	160 (98%)	3 (2%)	59	82
1	B	163/178 (92%)	161 (99%)	2 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	163/178 (92%)	161 (99%)	2 (1%)	71	88
1	D	163/178 (92%)	160 (98%)	3 (2%)	59	82
All	All	652/712 (92%)	642 (98%)	10 (2%)	65	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	95	LEU
1	A	136	PHE
1	B	95	LEU
1	B	144	ARG
1	C	95	LEU
1	C	162	ASP
1	D	136	PHE
1	D	186	LEU
1	D	188	ASP

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

Mol	Chain	Res	Type
1	C	143	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	199/213 (93%)	-0.14	0	100	100	52, 75, 107, 161	0
1	B	199/213 (93%)	-0.10	0	100	100	50, 75, 112, 149	0
1	C	199/213 (93%)	-0.13	0	100	100	58, 81, 112, 151	0
1	D	199/213 (93%)	0.02	1 (0%)	91	81	57, 103, 149, 176	0
All	All	796/852 (93%)	-0.09	1 (0%)	95	92	50, 80, 131, 176	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	GLY	2.8

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.