Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2021 – 05:10 am BST

PDB ID	:	7B5T
Title	:	S. agalactiae BusR transcription factor
Authors	:	Bandera, A.M.; Witte, G.
Deposited on	:	2020-12-07
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

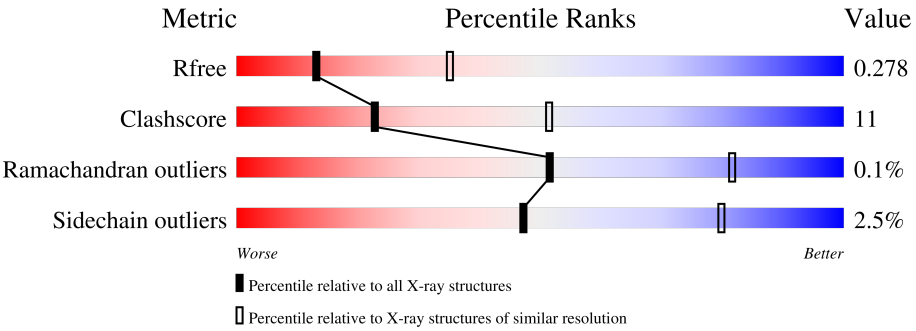
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Mol	Chain	Length	Quality of chain
1	A	215	73% 23%
1	B	215	76% 18%
1	C	215	70% 27%
1	D	215	67% 26% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6528 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 GntR family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	Se	0	0	0
			1656	1053	279	321	3			
1	B	207	Total	C	N	O	Se	0	0	0
			1628	1035	275	316	2			
1	D	200	Total	C	N	O	Se	0	0	0
			1573	1002	267	302	2			
1	C	210	Total	C	N	O	Se	0	0	0
			1649	1048	278	320	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP K0JNC6
A	0	PRO	-	expression tag	UNP K0JNC6
B	-1	GLY	-	expression tag	UNP K0JNC6
B	0	PRO	-	expression tag	UNP K0JNC6
D	-1	GLY	-	expression tag	UNP K0JNC6
D	0	PRO	-	expression tag	UNP K0JNC6
C	-1	GLY	-	expression tag	UNP K0JNC6
C	0	PRO	-	expression tag	UNP K0JNC6

- Molecule 2 is water.

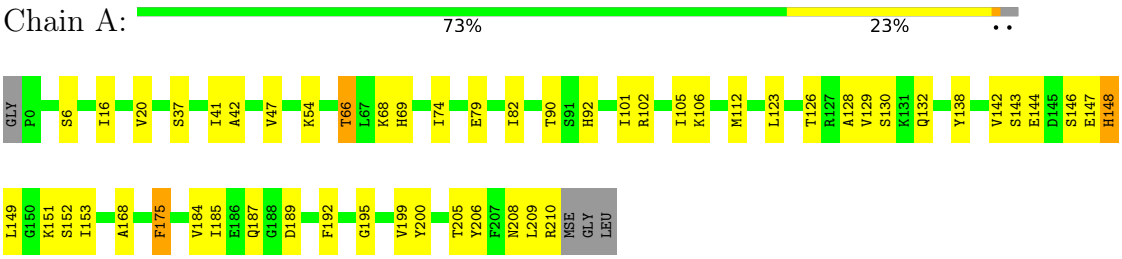
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	2	Total	O	0	0
			2	2		
2	D	5	Total	O	0	0
			5	5		
2	C	9	Total	O	0	0
			9	9		

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. 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. 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.

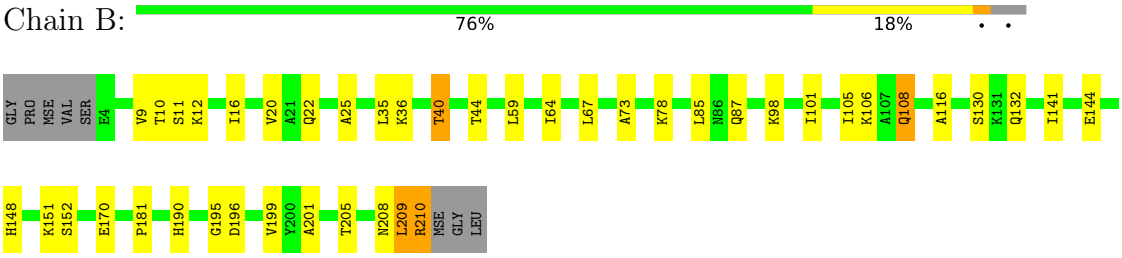
• Molecule 1: GntR family transcriptional regulator

Chain A:



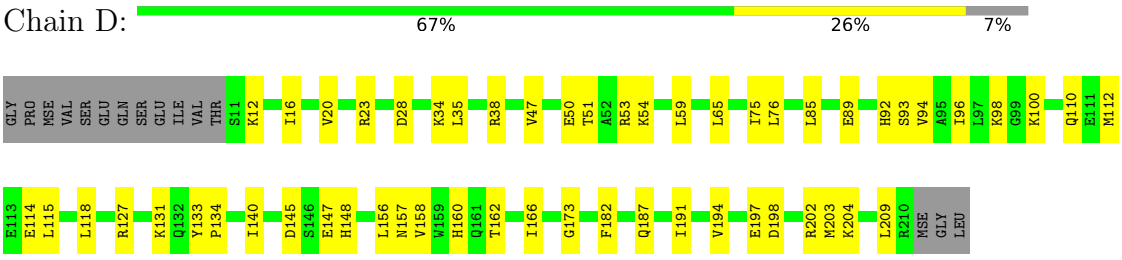
• Molecule 1: GntR family transcriptional regulator

Chain B:



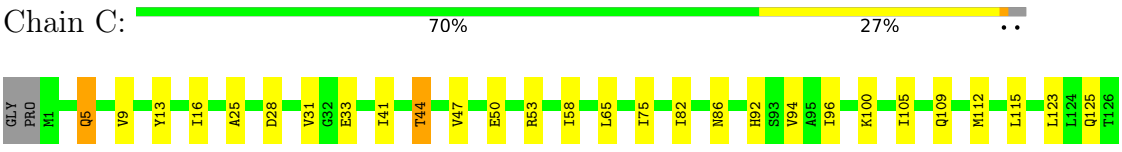
• Molecule 1: GntR family transcriptional regulator

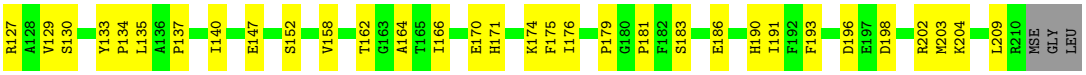
Chain D:



• Molecule 1: GntR family transcriptional regulator

Chain C:




R127
A128
V129
S130
Y133
P134
L135
A136
P137
I140
E147
S152
V158
T162
G163
A164
T165
I166
E170
H171
K174
F175
I176
P179
G180
P181
F182
S183
E186
H190
I191
F192
F193
D196
E197
D198
R202
M203
K204
L209
R210
MSE
GLY
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	114.18Å 114.18Å 240.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.80 44.32 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.22-2.80) 99.1 (44.32-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.257 , 0.269 0.257 , 0.278	Depositor DCC
R_{free} test set	1996 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å^2)	104.6	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6528	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.31	0/1681	0.54	0/2266
1	B	0.30	0/1653	0.52	0/2230
1	C	0.37	0/1674	0.60	1/2258 (0.0%)
1	D	0.33	0/1598	0.57	0/2155
All	All	0.33	0/6606	0.56	1/8909 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	5	GLN	N-CA-CB	-5.22	101.21	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	208	ASN	Mainchain

5.2 Too-close contacts

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	1656	0	1671	49	0
1	B	1628	0	1638	32	0
1	C	1649	0	1664	54	0
1	D	1573	0	1586	40	0
2	A	6	0	0	0	0
2	B	2	0	0	0	0
2	C	9	0	0	0	0
2	D	5	0	0	1	0
All	All	6528	0	6559	150	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 11.

All (150) 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:90:THR:HG23	1:A:92:HIS:H	1.37	0.88
1:A:147:GLU:HG2	1:A:148:HIS:H	1.42	0.85
1:C:204:LYS:HE2	1:C:209:LEU:HD23	1.65	0.77
1:C:13:TYR:HD1	1:C:58:ILE:HD11	1.49	0.77
1:C:198:ASP:O	1:C:202:ARG:HG3	1.87	0.73
1:C:50:GLU:OE2	1:C:53:ARG:NH1	2.22	0.73
1:D:89:GLU:OE1	1:C:129:VAL:HB	1.90	0.71
1:C:204:LYS:CE	1:C:209:LEU:HD23	2.20	0.71
1:D:23:ARG:NH2	1:C:137:PRO:O	2.25	0.70
1:C:170:GLU:HB3	1:C:190:HIS:HB2	1.73	0.69
1:C:13:TYR:CD1	1:C:58:ILE:HD11	2.27	0.68
1:A:105:ILE:HD13	1:B:116:ALA:HB2	1.78	0.66
1:D:85:LEU:HD22	1:C:130:SER:HB2	1.77	0.66
1:B:205:THR:HA	1:B:209:LEU:HB2	1.79	0.65
1:B:141:ILE:HG12	1:B:190:HIS:CD2	2.31	0.65
1:B:35:LEU:HD12	1:B:73:ALA:HB3	1.79	0.65
1:B:170:GLU:HB3	1:B:190:HIS:HB2	1.78	0.65
1:C:152:SER:HB2	1:C:181:PRO:O	1.97	0.65
1:D:148:HIS:HB3	1:D:156:LEU:HD11	1.79	0.63
1:C:204:LYS:CD	1:C:209:LEU:HD23	2.29	0.63
1:A:153:ILE:HD11	1:A:185:ILE:HD11	1.81	0.62
1:D:110:GLN:NE2	2:D:301:HOH:O	2.33	0.62
1:D:12:LYS:HD3	1:D:47:VAL:HG22	1.82	0.62
1:C:92:HIS:HD2	1:C:94:VAL:HG22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLU:HG2	1:A:148:HIS:N	2.12	0.62
1:A:168:ALA:HB1	1:A:175:PHE:HE1	1.65	0.61
1:A:142:VAL:HA	1:A:208:ASN:OD1	2.01	0.61
1:A:90:THR:HG23	1:A:92:HIS:N	2.15	0.60
1:C:171:HIS:HE1	1:C:186:GLU:HB2	1.66	0.60
1:C:204:LYS:HE2	1:C:209:LEU:CD2	2.31	0.60
1:A:144:GLU:OE1	1:A:187:GLN:NE2	2.21	0.59
1:D:112:MSE:SE	1:C:112:MSE:HG3	2.52	0.59
1:D:158:VAL:O	1:D:162:THR:HG22	2.02	0.59
1:A:200:TYR:HB3	1:C:125:GLN:HE21	1.67	0.59
1:C:105:ILE:HG23	1:C:109:GLN:HE22	1.68	0.58
1:A:42:ALA:HB1	1:A:47:VAL:O	2.04	0.58
1:A:153:ILE:CD1	1:A:185:ILE:HD11	2.34	0.58
1:C:204:LYS:HD2	1:C:209:LEU:HD23	1.86	0.58
1:C:16:ILE:HD11	1:C:47:VAL:HG21	1.85	0.57
1:A:147:GLU:OE1	1:A:147:GLU:N	2.38	0.57
1:D:23:ARG:NH1	1:D:28:ASP:OD2	2.38	0.57
1:A:168:ALA:HB2	1:C:135:LEU:HD21	1.87	0.56
1:C:152:SER:HA	1:C:183:SER:O	2.05	0.56
1:D:16:ILE:HD11	1:D:47:VAL:HG21	1.86	0.56
1:D:34:LYS:HG2	1:D:35:LEU:O	2.05	0.56
1:A:148:HIS:HB2	1:A:151:LYS:HD2	1.88	0.56
1:D:187:GLN:HG2	1:D:187:GLN:O	2.06	0.55
1:D:197:GLU:HG3	1:C:28:ASP:OD1	2.06	0.55
1:C:171:HIS:CE1	1:C:186:GLU:HB2	2.41	0.55
1:C:140:ILE:HG23	1:C:193:PHE:HE1	1.72	0.54
1:B:195:GLY:HA3	1:B:199:VAL:HG11	1.89	0.54
1:A:16:ILE:O	1:A:20:VAL:HG12	2.07	0.54
1:A:37:SER:O	1:A:41:ILE:HG13	2.08	0.54
1:A:123:LEU:HD22	1:B:98:LYS:HD3	1.88	0.54
1:A:105:ILE:HG13	1:A:106:LYS:N	2.22	0.53
1:A:147:GLU:HB3	1:A:210:ARG:HG2	1.90	0.53
1:B:22:GLN:HA	1:B:85:LEU:HD11	1.89	0.53
1:A:6:SER:HA	1:D:173:GLY:O	2.08	0.53
1:A:147:GLU:HA	1:A:210:ARG:NH2	2.23	0.53
1:C:133:TYR:N	1:C:134:PRO:HD2	2.24	0.53
1:D:162:THR:HG21	1:D:203:MSE:SE	2.59	0.52
1:A:66:THR:HG23	1:A:68:LYS:H	1.74	0.52
1:B:196:ASP:O	1:B:199:VAL:HG22	2.09	0.52
1:A:208:ASN:O	1:A:209:LEU:HD12	2.09	0.52
1:D:50:GLU:OE2	1:D:54:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:HD3	1:D:182:PHE:O	2.10	0.51
1:C:31:VAL:O	1:C:75:ILE:HB	2.10	0.51
1:C:179:PRO:HB2	1:C:183:SER:OG	2.11	0.51
1:A:200:TYR:CD1	1:C:125:GLN:HG2	2.46	0.50
1:B:105:ILE:HG13	1:B:106:LYS:N	2.26	0.50
1:C:96:ILE:O	1:C:100:LYS:HG3	2.11	0.50
1:C:162:THR:HG23	1:C:164:ALA:H	1.76	0.50
1:D:92:HIS:CD2	1:D:94:VAL:HG12	2.47	0.49
1:A:69:HIS:HD2	1:A:74:ILE:HD12	1.76	0.49
1:D:158:VAL:HG21	1:D:166:ILE:CD1	2.41	0.49
1:C:50:GLU:OE2	1:C:53:ARG:CZ	2.60	0.49
1:D:92:HIS:HD2	1:D:94:VAL:HG12	1.76	0.49
1:B:16:ILE:O	1:B:20:VAL:HG12	2.12	0.49
1:A:142:VAL:HG12	1:A:189:ASP:O	2.12	0.49
1:B:40:THR:O	1:B:44:THR:HG23	2.13	0.49
1:D:158:VAL:HG21	1:D:166:ILE:HD11	1.94	0.49
1:A:185:ILE:HD12	1:A:185:ILE:N	2.28	0.48
1:B:132:GLN:NE2	1:C:9:VAL:HG12	2.28	0.48
1:A:90:THR:HG21	1:B:201:ALA:HB1	1.96	0.48
1:A:147:GLU:OE2	1:A:206:TYR:O	2.32	0.48
1:B:101:ILE:O	1:B:105:ILE:HG23	2.14	0.48
1:A:208:ASN:C	1:A:209:LEU:HD12	2.33	0.48
1:A:90:THR:HG21	1:B:201:ALA:CB	2.44	0.47
1:D:114:GLU:O	1:D:118:LEU:HD13	2.14	0.47
1:B:25:ALA:O	1:B:78:LYS:HE3	2.14	0.47
1:C:140:ILE:HG13	1:C:191:ILE:HB	1.97	0.47
1:A:144:GLU:HA	1:A:187:GLN:NE2	2.29	0.46
1:A:101:ILE:HG23	1:D:115:LEU:HD11	1.97	0.46
1:A:168:ALA:HB3	1:A:192:PHE:HB2	1.96	0.46
1:D:133:TYR:CD1	1:D:134:PRO:HD3	2.50	0.46
1:D:157:ASN:HB3	1:D:160:HIS:HB3	1.97	0.46
1:B:101:ILE:HG23	1:C:115:LEU:HD11	1.97	0.46
1:A:102:ARG:HA	1:A:105:ILE:HG12	1.98	0.46
1:A:195:GLY:HA3	1:A:199:VAL:HG11	1.98	0.46
1:D:96:ILE:O	1:D:100:LYS:HG3	2.16	0.46
1:C:65:LEU:HD23	1:C:75:ILE:HA	1.97	0.46
1:C:133:TYR:H	1:C:134:PRO:HD2	1.81	0.46
1:C:33:GLU:O	1:C:75:ILE:HG12	2.16	0.45
1:D:133:TYR:N	1:D:134:PRO:HD2	2.30	0.45
1:D:147:GLU:HB3	1:D:148:HIS:H	1.50	0.45
1:B:36:LYS:HB3	1:B:40:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:O	1:A:82:ILE:HG12	2.17	0.45
1:A:123:LEU:CD2	1:B:98:LYS:HD3	2.45	0.45
1:A:149:LEU:H	1:A:149:LEU:HD23	1.81	0.45
1:C:65:LEU:HD21	1:C:75:ILE:HD13	1.99	0.45
1:C:158:VAL:O	1:C:162:THR:HG22	2.16	0.44
1:C:162:THR:HG21	1:C:203:MSE:SE	2.67	0.44
1:D:140:ILE:HD11	1:D:209:LEU:HD12	1.99	0.44
1:B:130:SER:HB2	1:D:127:ARG:NH1	2.32	0.44
1:D:47:VAL:HG12	1:D:51:THR:OG1	2.18	0.44
1:C:158:VAL:HG11	1:C:166:ILE:CD1	2.48	0.44
1:D:20:VAL:HG13	1:D:59:LEU:HD21	2.00	0.43
1:B:152:SER:HB2	1:B:181:PRO:O	2.19	0.43
1:B:12:LYS:HD3	1:B:12:LYS:HA	1.87	0.43
1:C:92:HIS:O	1:C:96:ILE:HG12	2.18	0.43
1:D:140:ILE:CG2	1:D:191:ILE:HB	2.48	0.43
1:B:148:HIS:HA	1:B:151:LYS:NZ	2.33	0.43
1:C:25:ALA:HB1	1:C:82:ILE:HG12	2.01	0.43
1:A:128:ALA:O	1:A:132:GLN:HG2	2.19	0.43
1:B:10:THR:OG1	1:B:11:SER:N	2.51	0.43
1:B:59:LEU:HD22	1:B:64:ILE:HD12	2.01	0.42
1:D:198:ASP:O	1:D:202:ARG:HG3	2.19	0.42
1:B:9:VAL:HG12	1:B:10:THR:O	2.19	0.42
1:D:93:SER:HA	1:D:96:ILE:HG12	2.00	0.42
1:D:140:ILE:HD11	1:D:204:LYS:HA	2.00	0.42
1:D:65:LEU:HA	1:D:76:LEU:HG	2.02	0.42
1:A:138:TYR:HE2	1:C:127:ARG:HH21	1.67	0.42
1:A:205:THR:HB	1:B:87:GLN:HE22	1.83	0.42
1:B:210:ARG:HD3	1:B:210:ARG:HA	1.95	0.42
1:B:209:LEU:HA	1:B:209:LEU:HD23	1.74	0.42
1:C:133:TYR:N	1:C:134:PRO:CD	2.83	0.42
1:D:38:ARG:HD2	1:D:53:ARG:HB2	2.00	0.41
1:A:101:ILE:O	1:A:105:ILE:HG23	2.20	0.41
1:A:143:SER:OG	1:A:144:GLU:N	2.53	0.41
1:C:133:TYR:CD2	1:C:134:PRO:HD3	2.56	0.41
1:C:162:THR:HG23	1:C:164:ALA:N	2.36	0.41
1:C:174:LYS:O	1:C:176:ILE:HD12	2.20	0.41
1:A:112:MSE:SE	1:B:108:GLN:HB3	2.70	0.41
1:B:209:LEU:HB3	1:B:210:ARG:H	1.55	0.41
1:A:130:SER:HA	1:C:127:ARG:NH1	2.35	0.41
1:C:41:ILE:HA	1:C:44:THR:OG1	2.21	0.41
1:A:126:THR:HA	1:A:129:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LYS:NZ	1:C:86:ASN:OD1	2.43	0.41
1:C:5:GLN:HG3	1:C:5:GLN:O	2.21	0.40
1:D:98:LYS:HG3	1:C:123:LEU:HD13	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	209/215 (97%)	196 (94%)	13 (6%)	0	100	100
1	B	205/215 (95%)	195 (95%)	9 (4%)	1 (0%)	29	61
1	C	208/215 (97%)	200 (96%)	8 (4%)	0	100	100
1	D	198/215 (92%)	189 (96%)	9 (4%)	0	100	100
All	All	820/860 (95%)	780 (95%)	39 (5%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	LEU

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	181/179 (101%)	175 (97%)	6 (3%)	38	72
1	B	177/179 (99%)	172 (97%)	5 (3%)	43	77
1	C	180/179 (101%)	176 (98%)	4 (2%)	52	83
1	D	170/179 (95%)	167 (98%)	3 (2%)	59	86
All	All	708/716 (99%)	690 (98%)	18 (2%)	47	80

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	146	SER
1	A	148	HIS
1	A	152	SER
1	A	175	PHE
1	A	184	VAL
1	B	40	THR
1	B	67	LEU
1	B	108	GLN
1	B	144	GLU
1	B	210	ARG
1	D	75	ILE
1	D	145	ASP
1	D	194	VAL
1	C	44	THR
1	C	147	GLU
1	C	175	PHE
1	C	196	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	87	GLN
1	A	110	GLN
1	B	87	GLN
1	B	148	HIS
1	B	157	ASN
1	B	160	HIS
1	B	171	HIS
1	D	14	GLN

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Mol	Chain	Res	Type
1	D	110	GLN
1	C	14	GLN
1	C	109	GLN
1	C	125	GLN
1	C	187	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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.