Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 05:04 AM EST

PDB ID	:	2OQT
Title	:	Structural Genomics, the crystal structure of a putative PTS IIA domain from Streptococcus pyogenes M1 GAS
Authors	:	Tan, K.; Wu, R.; Osipiuk, J.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2007-02-01
Resolution	:	2.41 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

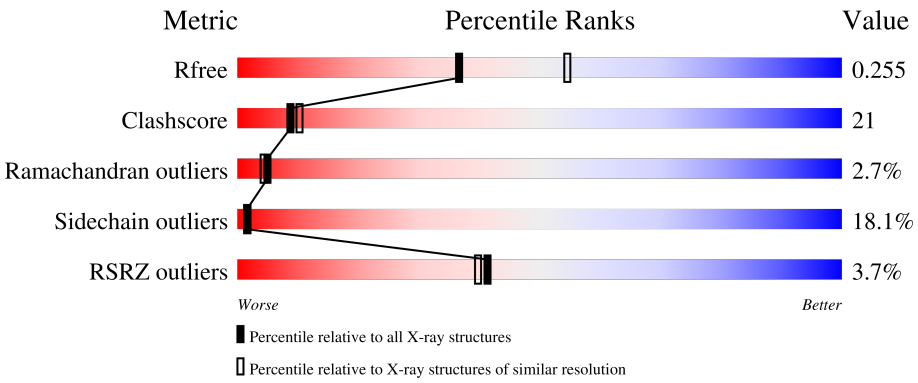
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	162	3% 54% 27% 12% • 7%
1	B	162	4% 54% 31% 6% • 7%
1	C	162	% 65% 21% 8% • 5%
1	D	162	6% 56% 31% 9% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4693 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 Hypothetical protein SPy0176.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	151	1154	735	189	224	1	5	0	1	0
1	B	151	1158	738	189	225	1	5	0	2	0
1	C	154	1175	750	189	230	1	5	0	1	0
1	D	156	1192	761	191	234	1	5	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	cloning artifact	UNP Q9A1N7
A	1	MSE	MET	modified residue	UNP Q9A1N7
A	7	LEU	PHE	SEE REMARK 999	UNP Q9A1N7
A	61	MSE	MET	modified residue	UNP Q9A1N7
A	64	MSE	MET	modified residue	UNP Q9A1N7
A	66	MSE	MET	modified residue	UNP Q9A1N7
A	144	MSE	MET	modified residue	UNP Q9A1N7
A	157	MSE	MET	modified residue	UNP Q9A1N7
B	0	ALA	-	cloning artifact	UNP Q9A1N7
B	1	MSE	MET	modified residue	UNP Q9A1N7
B	7	LEU	PHE	SEE REMARK 999	UNP Q9A1N7
B	61	MSE	MET	modified residue	UNP Q9A1N7
B	64	MSE	MET	modified residue	UNP Q9A1N7
B	66	MSE	MET	modified residue	UNP Q9A1N7
B	144	MSE	MET	modified residue	UNP Q9A1N7
B	157	MSE	MET	modified residue	UNP Q9A1N7
C	0	ALA	-	cloning artifact	UNP Q9A1N7
C	1	MSE	MET	modified residue	UNP Q9A1N7
C	7	LEU	PHE	SEE REMARK 999	UNP Q9A1N7
C	61	MSE	MET	modified residue	UNP Q9A1N7
C	64	MSE	MET	modified residue	UNP Q9A1N7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	66	MSE	MET	modified residue	UNP Q9A1N7
C	144	MSE	MET	modified residue	UNP Q9A1N7
C	157	MSE	MET	modified residue	UNP Q9A1N7
D	0	ALA	-	cloning artifact	UNP Q9A1N7
D	1	MSE	MET	modified residue	UNP Q9A1N7
D	7	LEU	PHE	SEE REMARK 999	UNP Q9A1N7
D	61	MSE	MET	modified residue	UNP Q9A1N7
D	64	MSE	MET	modified residue	UNP Q9A1N7
D	66	MSE	MET	modified residue	UNP Q9A1N7
D	144	MSE	MET	modified residue	UNP Q9A1N7
D	157	MSE	MET	modified residue	UNP Q9A1N7

- Molecule 2 is water.

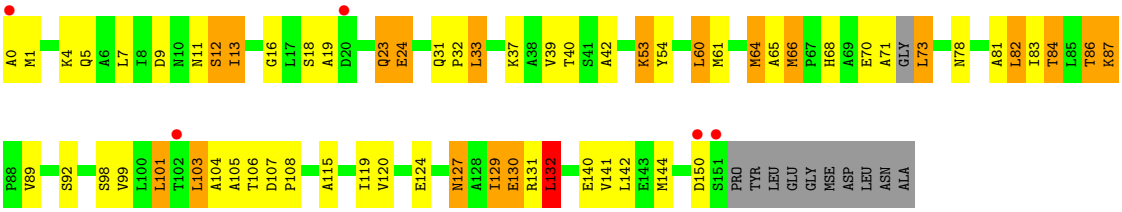
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	4	4	4	0	0
			Total	O		
2	B	3	3	3	0	0
			Total	O		
2	C	5	5	5	0	0
			Total	O		
2	D	2	2	2	0	0

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.

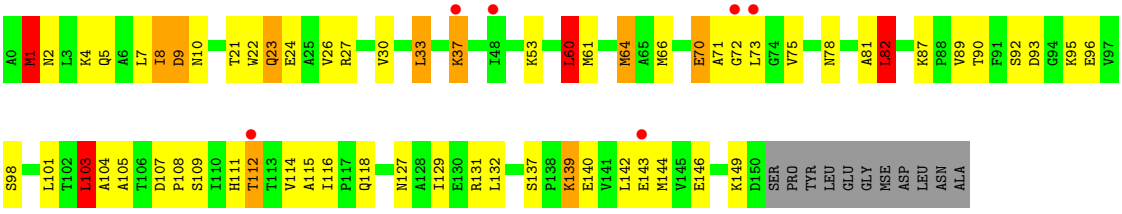
• Molecule 1: Hypothetical protein SPy0176

Chain A:



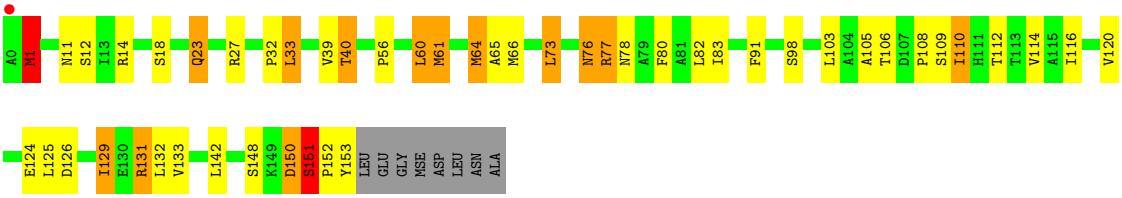
• Molecule 1: Hypothetical protein SPy0176

Chain B:



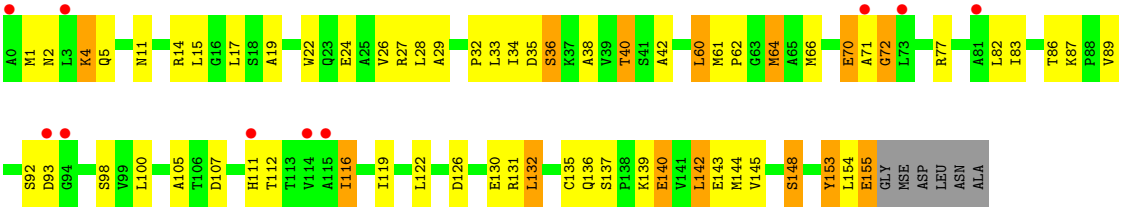
• Molecule 1: Hypothetical protein SPy0176

Chain C:



• Molecule 1: Hypothetical protein SPy0176

Chain D:


A0
M1
N2
L3
K4
Q5
N11
R14
L15
G16
L17
S18
A19
W22
Q23
E24
A25
V26
R27
L28
A29
P32
L33
I34
D35
S36
K37
A38
V39
T40
S41
A42
L60
M61
P62
G63
M64
A65
M66
E70
A71
G72
L73
R77
A81
L82
I83
T86
K87
P88
V89
S92
D93
G94
S98
V99
L100
A105
T106
D107
H111
T112
T113
V114
A115
I116
I119
L122
D126
E130
R131
L132
C135
Q136
S137
P138
K139
E140
V141
L142
E143
M144
V145
S148
Y153
L154
E155
GLY
MSE
ASP
LEU
ASN
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.22Å 112.78Å 60.40Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	35.85 – 2.41 35.84 – 2.41	Depositor EDS
% Data completeness (in resolution range)	90.1 (35.85-2.41) 90.1 (35.84-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.254 0.205 , 0.255	Depositor DCC
R_{free} test set	1196 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4693	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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 (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	0.82	0/1170	0.90	1/1585 (0.1%)
1	B	0.73	0/1178	0.87	3/1597 (0.2%)
1	C	0.83	0/1194	1.00	6/1621 (0.4%)
1	D	0.73	0/1210	0.85	1/1641 (0.1%)
All	All	0.78	0/4752	0.91	11/6444 (0.2%)

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	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	73	LEU	CA-CB-CG	8.47	134.79	115.30
1	C	151	SER	C-N-CD	-7.04	105.11	120.60
1	B	103	LEU	CA-CB-CG	6.74	130.81	115.30
1	B	82	LEU	CA-CB-CG	6.39	130.01	115.30
1	D	131	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	132	LEU	CA-CB-CG	5.81	128.66	115.30
1	C	151	SER	C-N-CA	5.53	145.21	122.00
1	C	151	SER	N-CA-C	5.48	125.79	111.00
1	C	1	MSE	CA-CB-CG	-5.29	104.30	113.30
1	C	1	MSE	N-CA-C	5.24	125.14	111.00
1	B	60	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	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	1154	0	1181	55	0
1	B	1158	0	1186	57	0
1	C	1175	0	1194	41	0
1	D	1192	0	1211	47	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	5	0	0	0	0
2	D	2	0	0	0	0
All	All	4693	0	4772	194	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 21.

All (194) 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:C:60:LEU:HB2	1:C:64:MSE:HE2	1.26	1.18
1:B:27[B]:ARG:HG2	1:B:27[B]:ARG:HH11	1.20	1.07
1:A:16:GLY:H	1:A:84:THR:HG22	1.25	1.00
1:D:60:LEU:HB2	1:D:64:MSE:HE2	1.44	0.99
1:A:107:ASP:OD1	1:A:108:PRO:HD2	1.66	0.95
1:B:27[B]:ARG:HH11	1:B:27[B]:ARG:CG	1.82	0.92
1:A:60:LEU:H	1:A:64:MSE:CE	1.82	0.92
1:B:61:MSE:H	1:B:64:MSE:HE2	1.34	0.92
1:A:68:HIS:HE1	1:B:112:THR:HG21	1.36	0.89
1:B:131:ARG:HB2	1:B:144:MSE:HE1	1.53	0.88
1:B:23:GLN:HE21	1:B:23:GLN:H	0.94	0.88
1:A:64:MSE:O	1:A:64:MSE:HE3	1.75	0.86
1:B:23:GLN:HE21	1:B:23:GLN:N	1.76	0.83
1:C:60:LEU:HB2	1:C:64:MSE:CE	2.07	0.83
1:C:64:MSE:HE3	1:C:65:ALA:CA	2.09	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:H	1:A:64:MSE:HE2	1.44	0.83
1:A:71:ALA:HB1	1:A:73:LEU:N	1.94	0.82
1:C:64:MSE:HE3	1:C:65:ALA:HA	1.61	0.81
1:B:60:LEU:H	1:B:64:MSE:CE	1.95	0.79
1:C:23:GLN:HE21	1:C:23:GLN:H	1.29	0.78
1:C:60:LEU:CB	1:C:64:MSE:HE2	2.11	0.78
1:A:130:GLU:H	1:A:130:GLU:CD	1.85	0.77
1:A:60:LEU:N	1:A:64:MSE:HE2	2.00	0.77
1:B:61:MSE:N	1:B:64:MSE:HE2	1.99	0.77
1:B:131:ARG:HB2	1:B:144:MSE:CE	2.16	0.76
1:B:93:ASP:OD2	1:B:95:LYS:HE2	1.87	0.75
1:B:78:ASN:HD22	1:B:105:ALA:HA	1.52	0.73
1:D:40:THR:HG22	1:D:42:ALA:H	1.54	0.73
1:B:23:GLN:H	1:B:23:GLN:NE2	1.78	0.72
1:B:127:ASN:O	1:B:131:ARG:HG3	1.90	0.71
1:C:129:ILE:O	1:C:133:VAL:HG23	1.91	0.71
1:A:40:THR:HG22	1:A:42:ALA:H	1.54	0.70
1:C:1:MSE:HG2	1:C:80:PHE:HE2	1.56	0.70
1:A:33:LEU:HD13	1:A:81:ALA:HB2	1.73	0.69
1:B:27[B]:ARG:HG2	1:B:27[B]:ARG:NH1	1.97	0.69
1:A:68:HIS:HE1	1:B:112:THR:CG2	2.06	0.68
1:A:16:GLY:N	1:A:84:THR:HG22	2.04	0.68
1:D:60:LEU:H	1:D:64:MSE:CE	2.07	0.68
1:C:120:VAL:O	1:C:124:GLU:HG2	1.93	0.68
1:B:78:ASN:ND2	1:B:105:ALA:HA	2.09	0.68
1:C:78:ASN:OD1	1:C:105:ALA:HA	1.94	0.67
1:D:34:ILE:C	1:D:36:SER:H	1.98	0.67
1:A:12:SER:HB3	1:A:81:ALA:HA	1.76	0.67
1:D:60:LEU:H	1:D:64:MSE:HE2	1.59	0.67
1:A:60:LEU:HD23	1:A:66:MSE:SE	2.44	0.67
1:D:22:TRP:HA	1:D:89:VAL:HG11	1.76	0.67
1:C:60:LEU:H	1:C:64:MSE:HE2	1.59	0.67
1:B:111:HIS:O	1:B:116:ILE:HG13	1.95	0.66
1:A:19:ALA:HB1	1:A:24:GLU:HB3	1.78	0.65
1:A:60:LEU:H	1:A:64:MSE:HE1	1.58	0.65
1:B:61:MSE:O	1:B:64:MSE:HG3	1.97	0.65
1:B:22:TRP:HA	1:B:89:VAL:HG11	1.79	0.65
1:A:23:GLN:H	1:A:23:GLN:HE21	1.46	0.64
1:D:83:ILE:HD11	1:D:100:LEU:HD13	1.79	0.64
1:C:66:MSE:O	1:C:66:MSE:HG3	1.98	0.64
1:A:101:LEU:HD22	1:A:119:ILE:CD1	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:H	1:C:23:GLN:NE2	1.96	0.63
1:A:103:LEU:C	1:A:103:LEU:HD23	2.19	0.62
1:A:78:ASN:ND2	1:A:106:THR:H	1.97	0.62
1:D:122:LEU:HA	1:D:148:SER:OG	1.98	0.62
1:C:1:MSE:HG2	1:C:80:PHE:CE2	2.33	0.62
1:B:66:MSE:CE	1:B:103:LEU:HD12	2.30	0.62
1:D:139:LYS:O	1:D:143[A]:GLU:HG3	2.00	0.62
1:C:64:MSE:HE3	1:C:65:ALA:N	2.14	0.62
1:A:132:LEU:HD13	1:A:144:MSE:SE	2.50	0.61
1:A:78:ASN:HD21	1:A:106:THR:H	1.45	0.61
1:B:2:ASN:HB3	1:B:5:GLN:HB2	1.81	0.61
1:B:24[B]:GLU:OE2	1:B:27[B]:ARG:NH1	2.34	0.61
1:C:152:PRO:HA	1:C:153:TYR:CD1	2.35	0.61
1:D:154:LEU:O	1:D:155:GLU:HB3	2.01	0.60
1:C:64:MSE:HE3	1:C:64:MSE:C	2.22	0.60
1:D:132:LEU:HD13	1:D:144:MSE:SE	2.52	0.60
1:C:151:SER:HB3	1:C:153:TYR:HA	1.84	0.59
1:A:70:GLU:HG3	1:B:109:SER:HB2	1.84	0.59
1:B:60:LEU:H	1:B:64:MSE:HE1	1.68	0.59
1:C:110:ILE:O	1:C:114:VAL:HG23	2.03	0.59
1:B:66:MSE:HE1	1:B:116:ILE:HG12	1.84	0.59
1:D:15:LEU:HD13	1:D:136:GLN:O	2.02	0.58
1:D:60:LEU:HB2	1:D:64:MSE:CE	2.28	0.58
1:D:60:LEU:CB	1:D:64:MSE:HE2	2.27	0.57
1:A:60:LEU:CD2	1:A:66:MSE:SE	3.02	0.57
1:D:40:THR:HG22	1:D:42:ALA:CB	2.34	0.57
1:D:40:THR:HG22	1:D:42:ALA:HB3	1.85	0.57
1:D:145:VAL:O	1:D:148:SER:HB2	2.05	0.57
1:B:27[B]:ARG:CG	1:B:27[B]:ARG:NH1	2.51	0.57
1:C:112:THR:O	1:C:116:ILE:HG12	2.04	0.57
1:B:8:ILE:O	1:B:10:ASN:N	2.38	0.56
1:B:33:LEU:HD13	1:B:81:ALA:HB2	1.87	0.56
1:A:64:MSE:HE3	1:A:65:ALA:HA	1.87	0.56
1:B:60:LEU:N	1:B:64:MSE:CE	2.68	0.55
1:D:64:MSE:O	1:D:64:MSE:HE3	2.06	0.55
1:A:86:THR:HG22	1:A:87:LYS:N	2.21	0.54
1:B:61:MSE:H	1:B:64:MSE:CE	2.16	0.54
1:A:64:MSE:CE	1:A:64:MSE:O	2.51	0.53
1:A:103:LEU:HD23	1:A:104:ALA:N	2.23	0.53
1:A:68:HIS:CE1	1:B:112:THR:HG21	2.28	0.53
1:C:60:LEU:H	1:C:64:MSE:CE	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ASP:H	1:D:111:HIS:HD2	1.58	0.52
1:D:34:ILE:O	1:D:36:SER:N	2.43	0.52
1:D:105:ALA:HB1	1:D:111:HIS:CD2	2.44	0.52
1:C:150:ASP:N	1:C:150:ASP:OD1	2.43	0.51
1:D:135:CYS:SG	1:D:140:GLU:HB2	2.50	0.51
1:B:60:LEU:HD11	1:B:66:MSE:SE	2.61	0.51
1:B:26:VAL:O	1:B:30:VAL:HG23	2.11	0.51
1:A:60:LEU:N	1:A:64:MSE:CE	2.58	0.51
1:D:19:ALA:HB1	1:D:24:GLU:HB3	1.93	0.51
1:D:40:THR:CG2	1:D:42:ALA:H	2.21	0.50
1:C:64:MSE:CE	1:C:65:ALA:CA	2.88	0.50
1:A:78:ASN:HD22	1:A:105:ALA:HA	1.76	0.50
1:C:76:ASN:O	1:C:77:ARG:CB	2.59	0.50
1:A:103:LEU:C	1:A:103:LEU:CD2	2.79	0.50
1:B:60:LEU:HD22	1:B:64:MSE:CE	2.42	0.50
1:A:61:MSE:H	1:A:64:MSE:HE2	1.78	0.49
1:A:78:ASN:ND2	1:A:105:ALA:HA	2.27	0.49
1:D:132:LEU:O	1:D:135:CYS:HB2	2.11	0.49
1:B:61:MSE:HG3	1:B:64:MSE:HG2	1.95	0.49
1:A:64:MSE:HE3	1:A:64:MSE:C	2.32	0.49
1:A:1:MSE:SE	1:A:78:ASN:HB3	2.63	0.48
1:C:108:PRO:O	1:C:112:THR:HG23	2.13	0.48
1:D:28:LEU:O	1:D:32:PRO:HD3	2.12	0.48
1:C:151:SER:HB3	1:C:153:TYR:CA	2.43	0.48
1:B:1:MSE:HE1	1:B:103:LEU:HD23	1.96	0.48
1:B:137:SER:OG	1:B:140:GLU:HG3	2.14	0.48
1:D:34:ILE:C	1:D:36:SER:N	2.62	0.48
1:D:24:GLU:HG3	1:D:27:ARG:HH12	1.79	0.48
1:D:71:ALA:O	1:D:72:GLY:C	2.51	0.48
1:B:21:THR:HB	1:B:23:GLN:NE2	2.29	0.47
1:C:1:MSE:SE	1:C:78:ASN:HB3	2.64	0.47
1:C:66:MSE:HE2	1:C:103:LEU:HB2	1.96	0.47
1:B:60:LEU:HD13	1:B:64:MSE:HE1	1.97	0.47
1:C:125:LEU:HB3	1:C:131:ARG:HH21	1.78	0.47
1:D:15:LEU:CD1	1:D:136:GLN:O	2.62	0.47
1:B:82:LEU:HB2	1:B:101:LEU:HG	1.97	0.46
1:C:12:SER:HA	1:C:32:PRO:HB3	1.98	0.46
1:C:64:MSE:CE	1:C:65:ALA:HA	2.41	0.46
1:A:5:GLN:NE2	1:A:9:ASP:OD1	2.49	0.46
1:C:61:MSE:CE	1:C:64:MSE:HG2	2.46	0.45
1:B:114:VAL:O	1:B:118:GLN:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HB3	1:A:32:PRO:HD3	1.99	0.45
1:D:4:LYS:HG2	1:D:142:LEU:HB2	1.98	0.45
1:B:8:ILE:HG22	1:B:9:ASP:N	2.32	0.45
1:D:107:ASP:H	1:D:111:HIS:CD2	2.35	0.45
1:A:13:ILE:HD13	1:A:141:VAL:HG11	1.99	0.44
1:A:120:VAL:O	1:A:124:GLU:HG3	2.17	0.44
1:D:60:LEU:HD22	1:D:64:MSE:HE1	1.98	0.44
1:B:70:GLU:OE1	1:B:73:LEU:HD23	2.17	0.44
1:B:139:LYS:O	1:B:143:GLU:HG3	2.18	0.44
1:C:33:LEU:HB3	1:C:39:VAL:HG22	1.99	0.44
1:A:66:MSE:HA	1:A:101:LEU:O	2.17	0.44
1:B:89:VAL:O	1:B:96:GLU:HA	2.17	0.44
1:B:107:ASP:OD1	1:B:108:PRO:HD2	2.17	0.44
1:D:2:ASN:HD22	1:D:5:GLN:H	1.66	0.43
1:D:22:TRP:O	1:D:26:VAL:HG23	2.17	0.43
1:D:29:ALA:HA	1:D:83:ILE:HG12	1.99	0.43
1:B:60:LEU:HD22	1:B:64:MSE:HE2	1.99	0.43
1:B:146:GLU:HA	1:B:149:LYS:HE3	2.00	0.43
1:C:76:ASN:O	1:C:77:ARG:HB3	2.17	0.43
1:A:53:LYS:HB2	1:A:53:LYS:HE2	1.74	0.43
1:D:71:ALA:HB2	1:D:105:ALA:O	2.18	0.43
1:C:125:LEU:HB3	1:C:131:ARG:NH2	2.34	0.43
1:A:64:MSE:HA	1:A:99:VAL:O	2.19	0.43
1:B:89:VAL:CG1	1:B:90:THR:N	2.82	0.43
1:D:14:ARG:HB3	1:D:17:LEU:HD21	2.00	0.43
1:A:53:LYS:HD3	1:A:54:TYR:CE2	2.53	0.42
1:B:8:ILE:O	1:B:9:ASP:C	2.58	0.42
1:C:56:PRO:HB3	1:C:91:PHE:HD1	1.84	0.42
1:A:98:SER:HB2	1:A:129:ILE:HD12	2.00	0.42
1:A:127:ASN:O	1:A:131:ARG:HG3	2.18	0.42
1:B:82:LEU:C	1:B:82:LEU:HD12	2.39	0.42
1:D:14:ARG:HB2	1:D:83:ILE:HG22	2.01	0.42
1:D:130:GLU:H	1:D:130:GLU:CD	2.22	0.42
1:D:64:MSE:HE3	1:D:64:MSE:C	2.38	0.42
1:C:60:LEU:N	1:C:64:MSE:HE2	2.29	0.42
1:D:66:MSE:HE3	1:D:119:ILE:HG12	2.01	0.42
1:A:82:LEU:HD12	1:A:83:ILE:N	2.35	0.42
1:D:112:THR:O	1:D:116:ILE:HD12	2.20	0.42
1:B:131:ARG:CB	1:B:144:MSE:HE1	2.36	0.41
1:A:130:GLU:OE1	1:A:130:GLU:N	2.52	0.41
1:D:38:ALA:HB2	1:D:77:ARG:NH2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:MSE:HE2	1:D:153:TYR:OH	2.20	0.41
1:D:60:LEU:HD22	1:D:64:MSE:CE	2.50	0.41
1:D:70:GLU:O	1:D:70:GLU:CG	2.69	0.41
1:C:14:ARG:O	1:C:83:ILE:HA	2.21	0.41
1:A:70:GLU:HA	1:A:70:GLU:OE1	2.20	0.41
1:A:86:THR:HG22	1:A:87:LYS:HB2	2.02	0.41
1:A:115:ALA:O	1:A:119:ILE:HG12	2.21	0.41
1:A:31:GLN:O	1:A:33:LEU:N	2.54	0.40
1:B:72:GLY:HA2	1:B:75:VAL:HB	2.03	0.40
1:B:78:ASN:HA	1:B:104:ALA:O	2.21	0.40
1:B:103:LEU:HG	1:B:115:ALA:HB1	2.02	0.40
1:A:33:LEU:HB3	1:A:39:VAL:HG22	2.04	0.40
1:A:92:SER:O	1:C:40:THR:HG21	2.21	0.40
1:B:66:MSE:HE3	1:B:66:MSE:HB2	1.97	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	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
1	B	151/162 (93%)	136 (90%)	7 (5%)	8 (5%)	2	1
1	C	153/162 (94%)	145 (95%)	6 (4%)	2 (1%)	12	16
1	D	155/162 (96%)	141 (91%)	8 (5%)	6 (4%)	3	2
All	All	607/648 (94%)	563 (93%)	28 (5%)	16 (3%)	5	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	77	ARG
1	B	9	ASP
1	B	70	GLU
1	B	71	ALA
1	B	92	SER
1	C	151	SER
1	D	72	GLY
1	D	92	SER
1	B	1	MSE
1	B	37	LYS
1	D	62	PRO
1	D	93	ASP
1	D	70	GLU
1	D	35	ASP
1	B	8	ILE

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	127/128 (99%)	98 (77%)	29 (23%)	1 1
1	B	127/128 (99%)	110 (87%)	17 (13%)	4 4
1	C	129/128 (101%)	105 (81%)	24 (19%)	1 1
1	D	131/128 (102%)	109 (83%)	22 (17%)	2 2
All	All	514/512 (100%)	422 (82%)	92 (18%)	1 2

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	LEU
1	A	11	ASN
1	A	12	SER
1	A	13	ILE
1	A	18	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	GLU
1	A	33	LEU
1	A	37	LYS
1	A	53	LYS
1	A	60	LEU
1	A	64	MSE
1	A	66	MSE
1	A	73	LEU
1	A	82	LEU
1	A	84	THR
1	A	86	THR
1	A	87	LYS
1	A	89	VAL
1	A	101	LEU
1	A	103	LEU
1	A	127	ASN
1	A	129	ILE
1	A	130	GLU
1	A	132	LEU
1	A	140	GLU
1	A	142	LEU
1	A	150	ASP
1	B	1	MSE
1	B	4	LYS
1	B	7	LEU
1	B	23	GLN
1	B	33	LEU
1	B	37	LYS
1	B	53	LYS
1	B	60	LEU
1	B	64	MSE
1	B	82	LEU
1	B	98	SER
1	B	103	LEU
1	B	112	THR
1	B	129	ILE
1	B	132	LEU
1	B	139	LYS
1	B	142	LEU
1	C	1	MSE
1	C	11	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	18	SER
1	C	23	GLN
1	C	27	ARG
1	C	33	LEU
1	C	40	THR
1	C	60	LEU
1	C	61	MSE
1	C	64	MSE
1	C	73	LEU
1	C	76	ASN
1	C	82	LEU
1	C	98	SER
1	C	106	THR
1	C	109	SER
1	C	110	ILE
1	C	126	ASP
1	C	129	ILE
1	C	131	ARG
1	C	132	LEU
1	C	142	LEU
1	C	148	SER
1	C	150	ASP
1	D	1	MSE
1	D	4	LYS
1	D	11	ASN
1	D	33	LEU
1	D	36	SER
1	D	40	THR
1	D	60	LEU
1	D	61	MSE
1	D	64	MSE
1	D	82	LEU
1	D	86	THR
1	D	87	LYS
1	D	98	SER
1	D	116	ILE
1	D	126	ASP
1	D	132	LEU
1	D	137	SER
1	D	140	GLU
1	D	142	LEU
1	D	148	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	153	TYR
1	D	155	GLU

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	11	ASN
1	A	23	GLN
1	A	31	GLN
1	A	68	HIS
1	A	78	ASN
1	B	23	GLN
1	B	78	ASN
1	B	127	ASN
1	C	23	GLN
1	C	127	ASN
1	D	2	ASN
1	D	5	GLN
1	D	11	ASN
1	D	111	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 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	146/162 (90%)	0.29	5 (3%)	45	43	48, 64, 84, 99	0
1	B	146/162 (90%)	0.24	6 (4%)	37	35	56, 74, 87, 93	0
1	C	149/162 (91%)	-0.26	1 (0%)	87	86	45, 60, 80, 90	0
1	D	151/162 (93%)	0.41	10 (6%)	18	16	59, 74, 88, 96	0
All	All	592/648 (91%)	0.17	22 (3%)	41	40	45, 69, 86, 99	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	SER	5.8
1	B	73	LEU	4.3
1	C	0	ALA	4.2
1	D	73	LEU	3.3
1	D	0	ALA	3.2
1	D	94	GLY	3.2
1	A	150	ASP	2.8
1	B	143	GLU	2.8
1	B	37	LYS	2.7
1	A	0	ALA	2.6
1	A	20	ASP	2.6
1	B	72	GLY	2.5
1	B	112	THR	2.5
1	B	48	ILE	2.4
1	D	114	VAL	2.3
1	A	102	THR	2.3
1	D	71	ALA	2.3
1	D	111	HIS	2.3
1	D	93	ASP	2.2
1	D	3	LEU	2.1
1	D	115	ALA	2.0
1	D	81	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.