Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 01:37 AM EDT

PDB ID	:	3C8G
Title	:	Crystal structure of a possible transciptional regulator YggD from Shigella flexneri 2a str. 2457T
Authors	:	Tan, K.; Borovilos, M.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-02-12
Resolution	:	2.50 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:

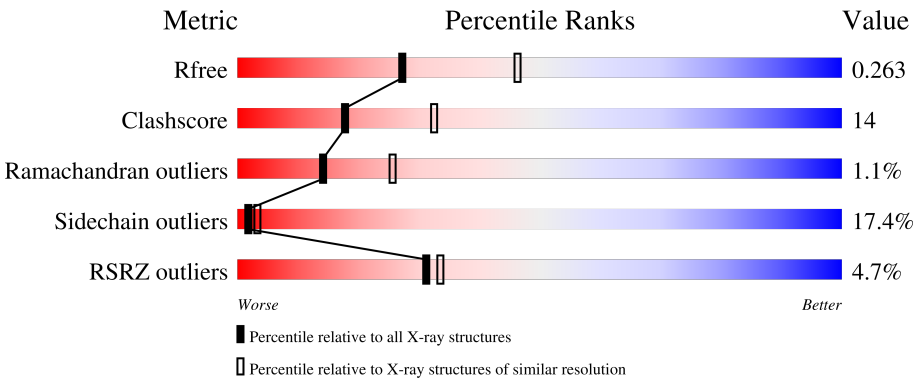
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	172	4% 60% 30% 6% •
1	C	172	2% 64% 27% 6% •
2	B	172	7% 57% 30% 9% •
3	D	172	3% 62% 23% 8% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5350 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 Putative transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	166	1341	869	209	258	5	0	0	0
1	C	167	1349	873	210	261	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q83Q96
A	-1	ASN	-	EXPRESSION TAG	UNP Q83Q96
A	0	ALA	-	EXPRESSION TAG	UNP Q83Q96
C	-2	SER	-	EXPRESSION TAG	UNP Q83Q96
C	-1	ASN	-	EXPRESSION TAG	UNP Q83Q96
C	0	ALA	-	EXPRESSION TAG	UNP Q83Q96

- Molecule 2 is a protein called Putative transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	B	166	1347	874	209	260	4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	EXPRESSION TAG	UNP Q83Q96
B	-1	ASN	-	EXPRESSION TAG	UNP Q83Q96
B	0	ALA	-	EXPRESSION TAG	UNP Q83Q96

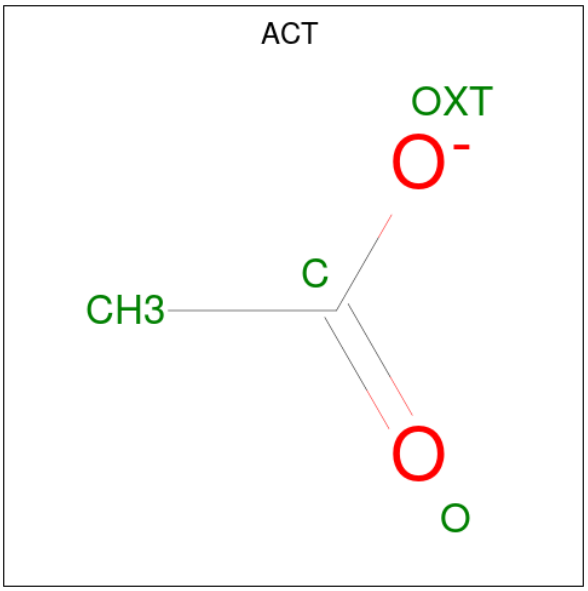
- Molecule 3 is a protein called Putative transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
3	D	161	1297	838	203	252	4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	EXPRESSION TAG	UNP Q83Q96
D	-1	ASN	-	EXPRESSION TAG	UNP Q83Q96
D	0	ALA	-	EXPRESSION TAG	UNP Q83Q96

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 is water.

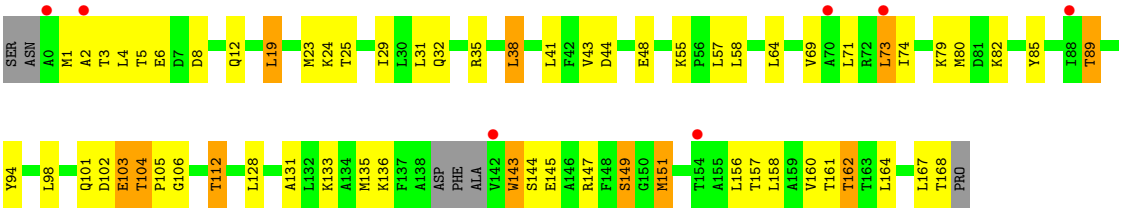
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	4	4	4	0	0
5	C	4	4	4	0	0
5	D	4	4	4	0	0

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.

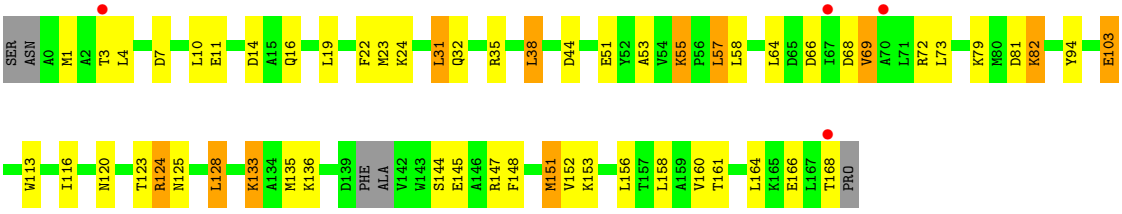
• Molecule 1: Putative transcriptional regulator

Chain A:



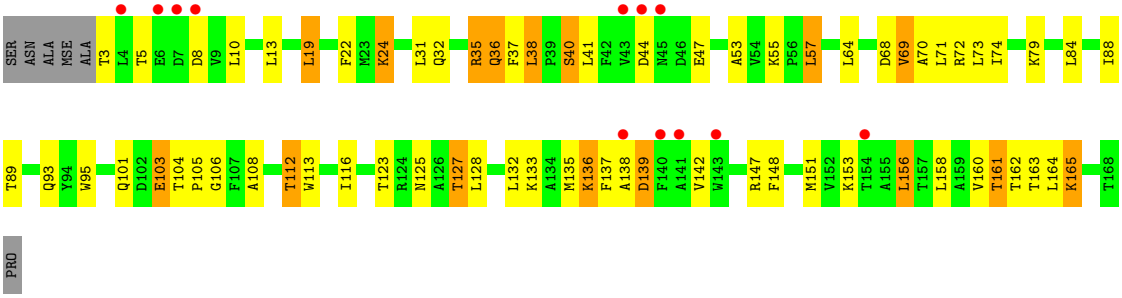
• Molecule 1: Putative transcriptional regulator

Chain C:



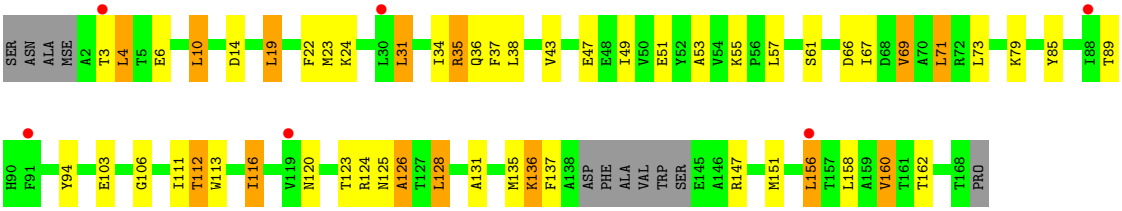
• Molecule 2: Putative transcriptional regulator

Chain B:



• Molecule 3: Putative transcriptional regulator

Chain D:


SER
ASN
ALA
MSE
A2
T3
L4
T5
E6
L10
D14
L19
F22
M23
K24
L30
L31
I34
R35
Q36
F37
L38
V43
E47
E48
I49
V50
E51
Y52
A53
V54
K55
P56
L57
S61
D66
I67
D68
V69
A70
L71
R72
L73
K79
Y85
I88
T89
H90
F91
Y94
E103
G106
I111
T112
W113
I116
V119
N120
T123
R124
N125
A126
T127
L128
A131
M135
K136
F137
A138
ASP
PHE
ALA
VAL
TRP
SER
E145
A146
R147
M151
L156
T157
L158
A159
V160
T161
T162
T168
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.36Å 70.95Å 159.04Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	31.81 – 2.50 31.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.9 (31.81-2.50) 93.9 (31.81-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.270 0.204 , 0.263	Depositor DCC
R_{free} test set	2020 reflections (7.74%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l 0.020 for -k,-h,-l 0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5350	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, ACT

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	0.76	0/1298	0.86	1/1765 (0.1%)
1	C	0.65	0/1306	0.74	0/1776
2	B	0.66	0/1307	0.79	0/1781
3	D	0.67	0/1275	0.82	0/1732
All	All	0.69	0/5186	0.80	1/7054 (0.0%)

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	A	73	LEU	CA-CB-CG	5.77	128.58	115.30

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	1341	0	1318	29	0
1	C	1349	0	1322	31	0
2	B	1347	0	1315	47	0
3	D	1297	0	1271	42	0
4	A	4	0	3	0	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4	0	0	0	0
5	D	4	0	0	0	0
All	All	5350	0	5229	144	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 (144) 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:135:MSE:HE1	1:C:151:MSE:HG3	1.40	1.04
2:B:35:ARG:HH21	2:B:35:ARG:HG2	1.33	0.92
1:A:151:MSE:SE	2:B:151:MSE:HE1	2.24	0.87
1:C:22:PHE:HD2	1:C:23:MSE:HE2	1.39	0.86
1:C:22:PHE:CD2	1:C:23:MSE:CE	2.59	0.85
1:C:22:PHE:CD2	1:C:23:MSE:HE2	2.15	0.82
1:C:16:GLN:O	1:C:153:LYS:HE3	1.79	0.82
3:D:135:MSE:SE	3:D:151:MSE:SE	2.98	0.81
1:C:22:PHE:HD2	1:C:23:MSE:CE	1.93	0.81
1:C:135:MSE:CE	1:C:151:MSE:HG3	2.11	0.79
2:B:132:LEU:HD11	2:B:151:MSE:HG3	1.65	0.78
1:A:1:MSE:HB2	1:A:32:GLN:HG3	1.65	0.78
2:B:132:LEU:CD1	2:B:151:MSE:HG3	2.13	0.77
1:A:19:LEU:HD22	1:A:23:MSE:HG2	1.67	0.74
1:A:167:LEU:O	1:A:168:THR:HG23	1.87	0.74
1:A:1:MSE:HE1	1:A:12:GLN:HE22	1.53	0.73
1:C:135:MSE:HE1	1:C:151:MSE:CG	2.17	0.73
2:B:106:GLY:O	2:B:112:THR:HG21	1.89	0.73
1:C:35:ARG:HA	1:C:38:LEU:HD22	1.70	0.73
3:D:31:LEU:HD22	3:D:35:ARG:HD2	1.71	0.72
2:B:35:ARG:HG2	2:B:35:ARG:NH2	2.00	0.72
1:C:58:LEU:HD23	1:C:64:LEU:HD12	1.70	0.72
1:A:98:LEU:HA	1:A:102:ASP:O	1.91	0.71
2:B:32:GLN:O	2:B:36:GLN:HG2	1.91	0.70
3:D:135:MSE:SE	3:D:151:MSE:HG3	2.43	0.68
1:C:22:PHE:CD2	1:C:23:MSE:HE3	2.28	0.67
3:D:106:GLY:O	3:D:112:THR:HG21	1.95	0.67
3:D:66:ASP:HB3	3:D:69:VAL:HG13	1.78	0.64
3:D:113:TRP:CE3	3:D:116:ILE:HD11	2.33	0.63
3:D:34:ILE:CD1	3:D:71:LEU:HD23	2.29	0.63
1:C:14:ASP:HA	1:C:153:LYS:NZ	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:O	1:C:35:ARG:HG3	1.98	0.62
2:B:125:ASN:OD1	2:B:127:THR:HG23	1.99	0.62
2:B:137:PHE:C	2:B:139:ASP:H	2.02	0.62
3:D:3:THR:HG23	3:D:36:GLN:HE22	1.63	0.61
2:B:35:ARG:HH21	2:B:35:ARG:CG	2.10	0.61
2:B:53:ALA:O	2:B:57:LEU:HB2	1.99	0.61
2:B:113:TRP:CE3	2:B:116:ILE:HD11	2.36	0.61
2:B:158:LEU:O	2:B:161:THR:HG22	2.00	0.61
3:D:4:LEU:H	3:D:4:LEU:HD13	1.65	0.61
1:A:85:TYR:O	1:A:89:THR:HG23	2.00	0.60
2:B:136:MLY:HB3	2:B:148:PHE:CE2	2.36	0.60
3:D:113:TRP:HA	3:D:116:ILE:HD13	1.83	0.60
3:D:34:ILE:HD11	3:D:71:LEU:HD23	1.84	0.59
3:D:131:ALA:O	3:D:135:MSE:HE3	2.02	0.59
1:C:14:ASP:HA	1:C:153:LYS:HZ3	1.68	0.59
3:D:67:ILE:O	3:D:71:LEU:HB2	2.03	0.58
1:C:53:ALA:O	1:C:57:LEU:HB2	2.03	0.58
1:A:131:ALA:HA	2:B:127:THR:OG1	2.03	0.58
2:B:32:GLN:OE1	2:B:35:ARG:HD3	2.04	0.57
1:C:135:MSE:SE	1:C:151:MSE:HG3	2.55	0.57
3:D:19:LEU:HD22	3:D:23:MSE:HG2	1.86	0.57
2:B:37:PHE:O	2:B:40:SER:HB2	2.04	0.56
2:B:158:LEU:O	2:B:162:THR:HG23	2.05	0.56
2:B:137:PHE:O	2:B:139:ASP:N	2.39	0.56
2:B:24:MLY:HD2	2:B:95:TRP:CH2	2.42	0.55
3:D:135:MSE:SE	3:D:151:MSE:CG	3.04	0.55
1:A:102:ASP:OD1	1:A:103:GLU:N	2.40	0.54
1:A:102:ASP:OD1	1:A:104:THR:OG1	2.24	0.54
3:D:125:ASN:OD1	3:D:128:LEU:HB2	2.06	0.54
2:B:106:GLY:O	2:B:112:THR:CG2	2.56	0.54
3:D:31:LEU:O	3:D:35:ARG:HG2	2.07	0.54
1:A:71:LEU:HD13	1:A:89:THR:HG22	1.90	0.53
1:A:151:MSE:HA	1:A:151:MSE:CE	2.39	0.52
3:D:113:TRP:CD2	3:D:136:MLY:HD2	2.45	0.52
1:C:66:ASP:HB3	1:C:69:VAL:CG1	2.40	0.52
1:C:22:PHE:CE2	1:C:23:MSE:CE	2.93	0.51
1:A:135:MSE:HE2	1:A:147:ARG:HD2	1.93	0.51
2:B:32:GLN:O	2:B:36:GLN:CG	2.59	0.51
3:D:23:MSE:HE2	3:D:94:TYR:HD1	1.76	0.51
3:D:53:ALA:O	3:D:57:LEU:HB2	2.10	0.51
3:D:94:TYR:OH	3:D:112:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:71:LEU:CD1	3:D:85:TYR:CD2	2.93	0.51
3:D:23:MSE:HE2	3:D:94:TYR:CD1	2.45	0.50
1:C:68:ASP:O	1:C:72:ARG:HG3	2.11	0.50
2:B:132:LEU:HD12	2:B:151:MSE:CG	2.42	0.50
1:A:151:MSE:HA	1:A:151:MSE:HE2	1.94	0.49
1:C:151:MSE:CE	3:D:135:MSE:HG3	2.42	0.49
1:A:106:GLY:O	1:A:112:THR:HG21	2.11	0.49
1:A:74:ILE:HG21	1:A:80:MSE:HE3	1.95	0.48
1:A:157:THR:HB	2:B:147:ARG:HH12	1.78	0.48
1:C:144:SER:OG	1:C:147:ARG:HB2	2.13	0.48
3:D:34:ILE:O	3:D:37:PHE:HB3	2.14	0.48
1:A:158:LEU:HD13	1:A:162:THR:CG2	2.44	0.47
1:A:35:ARG:HA	1:A:38:LEU:HD22	1.95	0.47
1:A:58:LEU:HD23	1:A:64:LEU:HD12	1.96	0.47
3:D:135:MSE:SE	3:D:151:MSE:HE3	2.64	0.47
1:A:104:THR:N	1:A:105:PRO:CD	2.76	0.47
1:A:145:GLU:O	1:A:149:SER:HB2	2.14	0.47
3:D:125:ASN:O	3:D:126:ALA:C	2.52	0.47
2:B:41:LEU:HD23	2:B:79:LYS:HD2	1.97	0.47
2:B:89:THR:O	2:B:93:GLN:HG3	2.15	0.47
2:B:132:LEU:CD1	2:B:151:MSE:CG	2.89	0.47
1:A:158:LEU:O	1:A:162:THR:CG2	2.63	0.47
2:B:13:LEU:HD22	2:B:22:PHE:CZ	2.50	0.47
3:D:71:LEU:HD12	3:D:85:TYR:CD2	2.50	0.47
3:D:120:ASN:O	3:D:124:ARG:HG3	2.14	0.47
2:B:142:VAL:CG1	2:B:142:VAL:O	2.63	0.46
2:B:137:PHE:C	2:B:139:ASP:N	2.68	0.46
2:B:24:MLY:HB3	2:B:95:TRP:CZ3	2.49	0.46
2:B:19:LEU:HD12	2:B:105:PRO:O	2.15	0.46
2:B:71:LEU:HD11	2:B:88:ILE:HG22	1.96	0.46
1:C:151:MSE:HE3	3:D:135:MSE:HE2	1.98	0.45
2:B:35:ARG:HA	2:B:38:LEU:HD22	1.97	0.45
2:B:132:LEU:HD12	2:B:151:MSE:HG3	1.95	0.45
3:D:22:PHE:CZ	3:D:156:LEU:HB3	2.51	0.45
2:B:104:THR:N	2:B:105:PRO:CD	2.80	0.45
3:D:113:TRP:CE2	3:D:136:MLY:HD2	2.52	0.45
3:D:156:LEU:O	3:D:160:VAL:HG12	2.17	0.44
3:D:106:GLY:O	3:D:112:THR:CG2	2.65	0.44
1:A:1:MSE:CE	1:A:12:GLN:HE22	2.25	0.44
3:D:34:ILE:HD13	3:D:71:LEU:HD23	1.99	0.44
1:C:120:ASN:O	1:C:124:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:71:LEU:HD12	3:D:85:TYR:CE2	2.52	0.44
2:B:70:ALA:O	2:B:74:ILE:HG13	2.18	0.43
1:C:103:GLU:H	1:C:103:GLU:HG3	1.19	0.43
3:D:136:MLY:HG3	3:D:137:PHE:CE2	2.53	0.43
2:B:68:ASP:HB3	2:B:72:ARG:HH21	1.83	0.43
1:C:1:MSE:HB2	1:C:32:GLN:HG3	1.99	0.43
3:D:71:LEU:HD22	3:D:71:LEU:HA	1.75	0.43
2:B:103:GLU:CD	2:B:103:GLU:H	2.22	0.43
2:B:5:THR:OG1	2:B:8:ASP:HB3	2.19	0.43
2:B:156:LEU:HD12	2:B:156:LEU:HA	1.93	0.43
3:D:43:VAL:HB	3:D:49:ILE:HG21	2.01	0.43
1:A:94:TYR:OH	1:A:112:THR:HG22	2.19	0.43
1:A:102:ASP:OD1	1:A:102:ASP:C	2.55	0.43
1:A:143:TRP:CG	1:A:144:SER:N	2.87	0.43
1:C:148:PHE:O	1:C:152:VAL:HG23	2.19	0.43
3:D:85:TYR:O	3:D:89:THR:HG23	2.19	0.42
2:B:135:MSE:HG2	2:B:148:PHE:HD2	1.83	0.42
1:C:51:GLU:OE2	1:C:55:MLY:HD3	2.19	0.42
2:B:165:MLY:HH22	2:B:165:MLY:HD2	1.83	0.42
1:A:43:VAL:CG1	1:A:44:ASP:N	2.83	0.42
2:B:64:LEU:HD23	2:B:69:VAL:HG23	2.01	0.42
2:B:84:LEU:HD11	2:B:163:THR:HG23	2.02	0.41
1:A:25:THR:HG22	1:A:29:ILE:HD12	2.02	0.41
2:B:24:MLY:HH22	2:B:24:MLY:HD3	1.79	0.41
1:C:82:MLY:HH22	1:C:82:MLY:HD3	1.91	0.41
3:D:10:LEU:O	3:D:14:ASP:HB2	2.21	0.41
1:C:113:TRP:CZ3	1:C:116:ILE:HD11	2.56	0.41
3:D:158:LEU:O	3:D:162:THR:HG23	2.20	0.41
2:B:108:ALA:O	2:B:136:MLY:HH11	2.21	0.41
1:C:133:MLY:HH22	1:C:133:MLY:HD3	1.90	0.41
1:C:125:ASN:HB3	1:C:128:LEU:HB3	2.03	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	156/172 (91%)	151 (97%)	4 (3%)	1 (1%)	25	43
1	C	157/172 (91%)	145 (92%)	9 (6%)	3 (2%)	8	13
2	B	158/172 (92%)	147 (93%)	10 (6%)	1 (1%)	25	43
3	D	153/172 (89%)	142 (93%)	9 (6%)	2 (1%)	12	21
All	All	624/688 (91%)	585 (94%)	32 (5%)	7 (1%)	14	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	138	ALA
1	A	2	ALA
1	C	3	THR
3	D	61	SER
1	C	123	THR
3	D	126	ALA
1	C	128	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	138/138 (100%)	111 (80%)	27 (20%)	1	2
1	C	139/138 (101%)	115 (83%)	24 (17%)	2	3
2	B	139/138 (101%)	115 (83%)	24 (17%)	2	3
3	D	136/140 (97%)	115 (85%)	21 (15%)	2	5
All	All	552/554 (100%)	456 (83%)	96 (17%)	2	3

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR

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Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	THR
1	A	6	GLU
1	A	8	ASP
1	A	19	LEU
1	A	31	LEU
1	A	38	LEU
1	A	41	LEU
1	A	48	GLU
1	A	57	LEU
1	A	69	VAL
1	A	73	LEU
1	A	89	THR
1	A	101	GLN
1	A	103	GLU
1	A	104	THR
1	A	112	THR
1	A	128	LEU
1	A	143	TRP
1	A	149	SER
1	A	151	MSE
1	A	156	LEU
1	A	160	VAL
1	A	161	THR
1	A	162	THR
1	A	164	LEU
2	B	3	THR
2	B	10	LEU
2	B	19	LEU
2	B	31	LEU
2	B	35	ARG
2	B	36	GLN
2	B	38	LEU
2	B	40	SER
2	B	44	ASP
2	B	47	GLU
2	B	57	LEU
2	B	69	VAL
2	B	73	LEU
2	B	101	GLN
2	B	103	GLU
2	B	112	THR

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Mol	Chain	Res	Type
2	B	123	THR
2	B	127	THR
2	B	128	LEU
2	B	139	ASP
2	B	156	LEU
2	B	160	VAL
2	B	161	THR
2	B	164	LEU
1	C	4	LEU
1	C	7	ASP
1	C	10	LEU
1	C	11	GLU
1	C	19	LEU
1	C	31	LEU
1	C	38	LEU
1	C	44	ASP
1	C	57	LEU
1	C	69	VAL
1	C	73	LEU
1	C	81	ASP
1	C	94	TYR
1	C	103	GLU
1	C	124	ARG
1	C	145	GLU
1	C	151	MSE
1	C	156	LEU
1	C	158	LEU
1	C	160	VAL
1	C	161	THR
1	C	164	LEU
1	C	166	GLU
1	C	168	THR
3	D	4	LEU
3	D	6	GLU
3	D	10	LEU
3	D	19	LEU
3	D	31	LEU
3	D	35	ARG
3	D	38	LEU
3	D	47	GLU
3	D	51	GLU
3	D	69	VAL

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Mol	Chain	Res	Type
3	D	71	LEU
3	D	73	LEU
3	D	103	GLU
3	D	111	ILE
3	D	112	THR
3	D	116	ILE
3	D	123	THR
3	D	128	LEU
3	D	147	ARG
3	D	156	LEU
3	D	160	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
2	B	45	ASN
2	B	99	ASN
1	C	99	ASN
3	D	32	GLN
3	D	36	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)

22 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MLY	B	133	2	9,10,11	0.47	0	6,11,13	2.29	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MLY	D	24	3	9,10,11	0.62	0	6,11,13	2.13	3 (50%)
1	MLY	A	79	1	9,10,11	0.69	0	6,11,13	2.00	3 (50%)
2	MLY	B	24	2	9,10,11	0.73	0	6,11,13	2.36	4 (66%)
1	MLY	A	55	1	9,10,11	0.53	0	6,11,13	2.78	4 (66%)
1	MLY	A	133	1	9,10,11	0.50	0	6,11,13	2.37	4 (66%)
1	MLY	C	24	1	9,10,11	0.31	0	6,11,13	2.15	2 (33%)
2	MLY	B	136	2	9,10,11	0.46	0	6,11,13	2.38	4 (66%)
3	MLY	D	55	3	9,10,11	0.82	0	6,11,13	2.03	2 (33%)
1	MLY	A	82	1	9,10,11	0.53	0	6,11,13	2.35	4 (66%)
1	MLY	C	79	1	9,10,11	0.44	0	6,11,13	2.27	3 (50%)
1	MLY	C	136	1	9,10,11	0.46	0	6,11,13	2.58	4 (66%)
2	MLY	B	153	2	9,10,11	0.63	0	6,11,13	2.35	3 (50%)
1	MLY	A	136	1	9,10,11	0.56	0	6,11,13	2.63	5 (83%)
1	MLY	C	55	1	9,10,11	0.50	0	6,11,13	2.23	4 (66%)
1	MLY	C	133	1	9,10,11	0.44	0	6,11,13	2.11	2 (33%)
2	MLY	B	55	2	9,10,11	0.52	0	6,11,13	2.02	3 (50%)
2	MLY	B	165	2	9,10,11	0.58	0	6,11,13	2.19	3 (50%)
1	MLY	C	82	1	9,10,11	0.49	0	6,11,13	2.09	3 (50%)
3	MLY	D	136	3	9,10,11	0.53	0	6,11,13	2.50	4 (66%)
3	MLY	D	79	3	9,10,11	0.68	0	6,11,13	2.05	3 (50%)
1	MLY	A	24	1	9,10,11	0.56	0	6,11,13	2.27	4 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	133	2	-	3/8/9/11	-
3	MLY	D	24	3	-	1/8/9/11	-
1	MLY	A	79	1	-	4/8/9/11	-
2	MLY	B	24	2	-	7/8/9/11	-
1	MLY	A	55	1	-	4/8/9/11	-
1	MLY	A	133	1	-	1/8/9/11	-
1	MLY	C	24	1	-	2/8/9/11	-
2	MLY	B	136	2	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLY	D	55	3	-	6/8/9/11	-
1	MLY	A	82	1	-	3/8/9/11	-
1	MLY	C	79	1	-	3/8/9/11	-
1	MLY	C	136	1	-	2/8/9/11	-
2	MLY	B	153	2	-	3/8/9/11	-
1	MLY	A	136	1	-	4/8/9/11	-
1	MLY	C	55	1	-	2/8/9/11	-
1	MLY	C	133	1	-	4/8/9/11	-
2	MLY	B	55	2	-	2/8/9/11	-
2	MLY	B	165	2	-	5/8/9/11	-
1	MLY	C	82	1	-	4/8/9/11	-
3	MLY	D	136	3	-	5/8/9/11	-
3	MLY	D	79	3	-	5/8/9/11	-
1	MLY	A	24	1	-	1/8/9/11	-

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	MLY	CH2-NZ-CH1	4.89	122.26	109.72
1	C	136	MLY	CH2-NZ-CH1	4.13	120.30	109.72
2	B	153	MLY	CH2-NZ-CH1	4.13	120.30	109.72
1	C	79	MLY	CH2-NZ-CH1	4.12	120.27	109.72
1	A	136	MLY	CH2-NZ-CH1	4.05	120.10	109.72
2	B	24	MLY	CH2-NZ-CH1	4.03	120.05	109.72
1	A	133	MLY	CH2-NZ-CH1	3.98	119.93	109.72
3	D	136	MLY	CH2-NZ-CH1	3.92	119.77	109.72
1	A	82	MLY	CH2-NZ-CH1	3.80	119.47	109.72
2	B	133	MLY	CH2-NZ-CH1	3.79	119.44	109.72
2	B	165	MLY	CH2-NZ-CH1	3.77	119.37	109.72
2	B	136	MLY	CH2-NZ-CH1	3.75	119.34	109.72
1	C	55	MLY	CH2-NZ-CH1	3.51	118.72	109.72
1	C	24	MLY	CH2-NZ-CH1	3.46	118.58	109.72
1	A	24	MLY	CH2-NZ-CH1	3.43	118.52	109.72
1	C	82	MLY	CH2-NZ-CH1	3.42	118.49	109.72
1	C	136	MLY	CD-CE-NZ	-3.41	104.91	113.71
3	D	55	MLY	CH1-NZ-CE	3.32	123.93	110.75
3	D	136	MLY	CD-CE-NZ	-3.28	105.23	113.71
1	C	133	MLY	CH2-NZ-CE	3.27	123.73	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	55	MLY	CH2-NZ-CH1	3.23	117.99	109.72
1	C	24	MLY	CH2-NZ-CE	3.21	123.50	110.75
1	C	133	MLY	CH2-NZ-CH1	3.13	117.74	109.72
3	D	24	MLY	CH2-NZ-CH1	3.13	117.74	109.72
3	D	55	MLY	CH2-NZ-CH1	3.05	117.54	109.72
1	A	55	MLY	CD-CE-NZ	-3.04	105.87	113.71
1	A	136	MLY	CD-CE-NZ	-3.02	105.92	113.71
3	D	79	MLY	CH1-NZ-CE	3.02	122.70	110.75
1	A	24	MLY	CH1-NZ-CE	3.00	122.64	110.75
3	D	79	MLY	CH2-NZ-CH1	2.94	117.26	109.72
2	B	55	MLY	CH2-NZ-CE	2.94	122.39	110.75
1	C	55	MLY	CH1-NZ-CE	2.92	122.34	110.75
1	A	79	MLY	CH2-NZ-CE	2.90	122.27	110.75
2	B	133	MLY	CH2-NZ-CE	2.89	122.20	110.75
2	B	136	MLY	CD-CE-NZ	-2.82	106.42	113.71
1	C	82	MLY	CH2-NZ-CE	2.80	121.85	110.75
1	A	79	MLY	CH2-NZ-CH1	2.77	116.83	109.72
3	D	24	MLY	CH2-NZ-CE	2.76	121.71	110.75
2	B	136	MLY	CH1-NZ-CE	2.70	121.46	110.75
2	B	165	MLY	CH2-NZ-CE	2.68	121.37	110.75
1	A	82	MLY	CH2-NZ-CE	2.59	121.04	110.75
1	C	136	MLY	CH2-NZ-CE	2.58	120.99	110.75
1	A	133	MLY	CD-CE-NZ	-2.57	107.06	113.71
1	A	79	MLY	CH1-NZ-CE	2.56	120.91	110.75
2	B	24	MLY	CH2-NZ-CE	2.55	120.88	110.75
1	A	82	MLY	CD-CE-NZ	-2.55	107.12	113.71
1	C	79	MLY	CH1-NZ-CE	2.53	120.78	110.75
1	A	133	MLY	CH1-NZ-CE	2.47	120.53	110.75
3	D	24	MLY	CH1-NZ-CE	2.46	120.52	110.75
3	D	136	MLY	CH2-NZ-CE	2.39	120.23	110.75
2	B	153	MLY	CH2-NZ-CE	2.38	120.17	110.75
1	A	136	MLY	CH1-NZ-CE	2.34	120.04	110.75
3	D	79	MLY	CH2-NZ-CE	2.34	120.03	110.75
2	B	24	MLY	CD-CE-NZ	-2.34	107.67	113.71
3	D	136	MLY	CH1-NZ-CE	2.33	120.00	110.75
1	A	136	MLY	CH2-NZ-CE	2.29	119.85	110.75
1	A	55	MLY	CH1-NZ-CE	2.29	119.83	110.75
1	C	82	MLY	CH1-NZ-CE	2.25	119.67	110.75
2	B	55	MLY	CH1-NZ-CE	2.24	119.62	110.75
1	A	133	MLY	CH2-NZ-CE	2.22	119.54	110.75
2	B	153	MLY	CH1-NZ-CE	2.21	119.53	110.75
1	A	82	MLY	CH1-NZ-CE	2.21	119.50	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	MLY	CD-CG-CB	-2.17	105.43	113.62
1	A	136	MLY	CG-CD-CE	-2.17	103.32	113.17
1	C	55	MLY	CD-CE-NZ	-2.16	108.13	113.71
2	B	165	MLY	CH1-NZ-CE	2.14	119.25	110.75
2	B	136	MLY	CH2-NZ-CE	2.13	119.18	110.75
2	B	24	MLY	CH1-NZ-CE	2.10	119.07	110.75
1	C	79	MLY	CH2-NZ-CE	2.06	118.94	110.75
1	C	55	MLY	CH2-NZ-CE	2.06	118.93	110.75
2	B	133	MLY	CD-CE-NZ	-2.06	108.38	113.71
1	A	24	MLY	CG-CD-CE	-2.05	103.84	113.17
1	A	24	MLY	CH2-NZ-CE	2.01	118.72	110.75
1	C	136	MLY	CH1-NZ-CE	2.01	118.71	110.75

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	55	MLY	N-CA-CB-CG
1	A	55	MLY	C-CA-CB-CG
1	A	79	MLY	O-C-CA-CB
1	A	136	MLY	O-C-CA-CB
2	B	24	MLY	C-CA-CB-CG
2	B	133	MLY	C-CA-CB-CG
2	B	136	MLY	O-C-CA-CB
1	C	133	MLY	C-CA-CB-CG
1	C	136	MLY	C-CA-CB-CG
3	D	55	MLY	C-CA-CB-CG
3	D	79	MLY	O-C-CA-CB
3	D	136	MLY	C-CA-CB-CG
1	A	55	MLY	CD-CE-NZ-CH2
1	A	79	MLY	CD-CE-NZ-CH1
1	A	82	MLY	CD-CE-NZ-CH1
1	A	136	MLY	CD-CE-NZ-CH2
2	B	133	MLY	CD-CE-NZ-CH1
2	B	136	MLY	CD-CE-NZ-CH2
1	C	55	MLY	CD-CE-NZ-CH1
1	C	79	MLY	CD-CE-NZ-CH2
3	D	24	MLY	CD-CE-NZ-CH2
3	D	79	MLY	CD-CE-NZ-CH2
3	D	79	MLY	CG-CD-CE-NZ
2	B	165	MLY	CG-CD-CE-NZ
3	D	136	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
2	B	24	MLY	CG-CD-CE-NZ
2	B	24	MLY	CD-CE-NZ-CH1
2	B	55	MLY	CD-CE-NZ-CH2
2	B	153	MLY	CD-CE-NZ-CH2
1	C	136	MLY	CD-CE-NZ-CH1
3	D	136	MLY	CD-CE-NZ-CH1
1	C	82	MLY	CG-CD-CE-NZ
3	D	55	MLY	CG-CD-CE-NZ
1	A	24	MLY	CD-CE-NZ-CH1
2	B	165	MLY	CD-CE-NZ-CH2
1	C	82	MLY	CD-CE-NZ-CH2
1	C	133	MLY	CD-CE-NZ-CH2
1	C	133	MLY	CG-CD-CE-NZ
1	C	24	MLY	CD-CE-NZ-CH2
3	D	55	MLY	CD-CE-NZ-CH1
2	B	24	MLY	CD-CE-NZ-CH2
2	B	165	MLY	CA-CB-CG-CD
1	C	79	MLY	CE-CD-CG-CB
2	B	153	MLY	CG-CD-CE-NZ
2	B	153	MLY	CE-CD-CG-CB
2	B	24	MLY	CE-CD-CG-CB
3	D	79	MLY	CE-CD-CG-CB
1	A	133	MLY	CD-CE-NZ-CH2
2	B	165	MLY	CD-CE-NZ-CH1
2	B	24	MLY	CA-CB-CG-CD
1	A	55	MLY	CG-CD-CE-NZ
1	C	79	MLY	CG-CD-CE-NZ
1	A	79	MLY	CG-CD-CE-NZ
1	A	136	MLY	CE-CD-CG-CB
1	A	79	MLY	CA-CB-CG-CD
3	D	79	MLY	CA-CB-CG-CD
3	D	136	MLY	CA-CB-CG-CD
3	D	55	MLY	CA-CB-CG-CD
1	A	82	MLY	CG-CD-CE-NZ
3	D	55	MLY	CE-CD-CG-CB
2	B	24	MLY	N-CA-CB-CG
2	B	133	MLY	N-CA-CB-CG
1	C	82	MLY	N-CA-CB-CG
3	D	55	MLY	N-CA-CB-CG
3	D	136	MLY	N-CA-CB-CG
1	A	82	MLY	CE-CD-CG-CB
2	B	165	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	C	24	MLY	CE-CD-CG-CB
1	C	55	MLY	CD-CE-NZ-CH2
2	B	55	MLY	C-CA-CB-CG
2	B	136	MLY	CG-CD-CE-NZ
1	C	133	MLY	CE-CD-CG-CB
1	C	82	MLY	CA-CB-CG-CD
1	A	136	MLY	CD-CE-NZ-CH1

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	24	MLY	3	0
2	B	136	MLY	2	0
1	C	55	MLY	1	0
1	C	133	MLY	1	0
2	B	165	MLY	1	0
1	C	82	MLY	1	0
3	D	136	MLY	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	A	201	-	3,3,3	0.80	0	3,3,3	1.33	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	155/172 (90%)	0.28	7 (4%)	33	36	51, 61, 83, 96	0
1	C	156/172 (90%)	0.18	4 (2%)	56	59	51, 62, 86, 107	0
2	B	156/172 (90%)	0.34	12 (7%)	13	13	54, 63, 85, 90	0
3	D	153/172 (88%)	0.31	6 (3%)	39	42	52, 62, 76, 89	0
All	All	620/688 (90%)	0.28	29 (4%)	31	33	51, 62, 83, 107	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	140	PHE	5.2
2	B	141	ALA	3.7
1	A	142	VAL	3.7
2	B	4	LEU	3.5
2	B	138	ALA	3.4
3	D	156	LEU	3.3
2	B	143	TRP	3.2
3	D	91	PHE	3.1
1	C	168	THR	3.0
1	A	2	ALA	3.0
3	D	3	THR	2.8
3	D	88	ILE	2.8
1	C	3	THR	2.7
1	A	0	ALA	2.6
1	C	70	ALA	2.6
1	A	88	ILE	2.5
2	B	8	ASP	2.4
3	D	30	LEU	2.3
1	A	154	THR	2.3
2	B	45	ASN	2.2
1	A	70	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	119	VAL	2.2
1	C	67	ILE	2.1
2	B	44	ASP	2.1
2	B	7	ASP	2.1
2	B	154	THR	2.1
1	A	73	LEU	2.1
2	B	43	VAL	2.1
2	B	6	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLY	B	165	11/12	0.84	0.32	70,72,80,81	0
1	MLY	C	82	11/12	0.89	0.32	64,65,70,71	0
2	MLY	B	55	11/12	0.91	0.23	58,59,69,70	0
3	MLY	D	79	11/12	0.91	0.22	57,60,65,65	0
1	MLY	A	55	11/12	0.93	0.18	53,56,69,69	0
1	MLY	C	133	11/12	0.93	0.12	62,64,69,69	0
1	MLY	C	136	11/12	0.93	0.17	69,70,75,76	0
3	MLY	D	55	11/12	0.93	0.23	54,57,70,70	0
1	MLY	A	82	11/12	0.93	0.21	64,66,78,78	0
2	MLY	B	153	11/12	0.94	0.28	59,61,77,78	0
1	MLY	A	133	11/12	0.94	0.17	53,54,57,58	0
1	MLY	C	79	11/12	0.94	0.18	62,65,74,74	0
1	MLY	A	79	11/12	0.94	0.13	64,64,66,66	0
2	MLY	B	136	11/12	0.95	0.14	69,73,76,76	0
1	MLY	C	24	11/12	0.95	0.17	44,49,55,56	0
2	MLY	B	24	11/12	0.96	0.17	58,59,62,65	0
1	MLY	C	55	11/12	0.96	0.15	52,54,58,60	0
3	MLY	D	24	11/12	0.96	0.23	54,58,60,61	0
1	MLY	A	136	11/12	0.96	0.15	61,62,71,73	0
2	MLY	B	133	11/12	0.96	0.14	59,61,67,68	0
3	MLY	D	136	11/12	0.96	0.18	61,63,65,65	0
1	MLY	A	24	11/12	0.97	0.18	52,54,56,56	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	A	201	4/4	0.92	0.15	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.