Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 08:43 AM EDT

PDB ID	:	2PQQ
Title	:	Structural Genomics, the crystal structure of the N-terminal domain of a transcriptional regulator from Streptomyces coelicolor A3(2)
Authors	:	Tan, K.; Xu, X.; Zheng, H.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2007-05-02
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

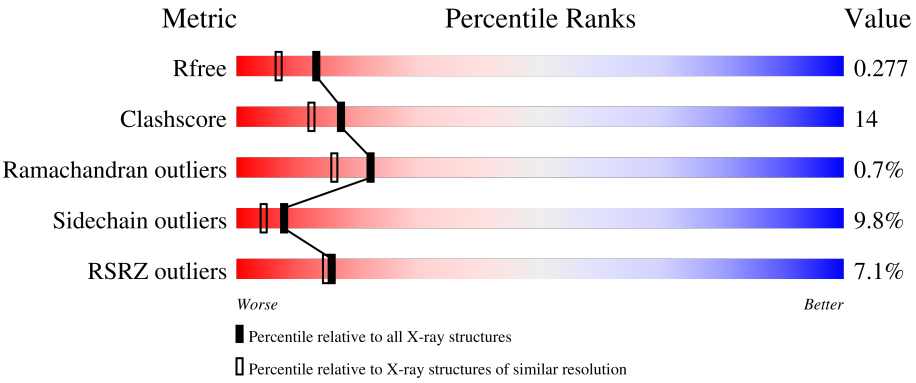
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	149	8% 70% 23% 5% •
1	B	149	5% 75% 15% 6% •
1	C	149	5% 72% 19% • 6%
1	D	149	8% 68% 21% 5% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4667 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
1	A	147	Total	C	N	O	Se	0	1	0
			1130	701	208	217	4			
1	B	144	Total	C	N	O	Se	0	1	0
			1104	680	203	217	4			
1	C	140	Total	C	N	O	Se	0	0	0
			1067	660	196	208	3			
1	D	143	Total	C	N	O	Se	0	2	0
			1106	688	202	213	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9XA42
A	0	HIS	-	CLONING ARTIFACT	UNP Q9XA42
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
A	26	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
A	68	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
A	138	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
A	146	GLY	-	CLONING ARTIFACT	UNP Q9XA42
A	147	SER	-	CLONING ARTIFACT	UNP Q9XA42
B	-1	GLY	-	CLONING ARTIFACT	UNP Q9XA42
B	0	HIS	-	CLONING ARTIFACT	UNP Q9XA42
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
B	26	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
B	68	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
B	138	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
B	146	GLY	-	CLONING ARTIFACT	UNP Q9XA42
B	147	SER	-	CLONING ARTIFACT	UNP Q9XA42
C	-1	GLY	-	CLONING ARTIFACT	UNP Q9XA42
C	0	HIS	-	CLONING ARTIFACT	UNP Q9XA42
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
C	26	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
C	68	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42

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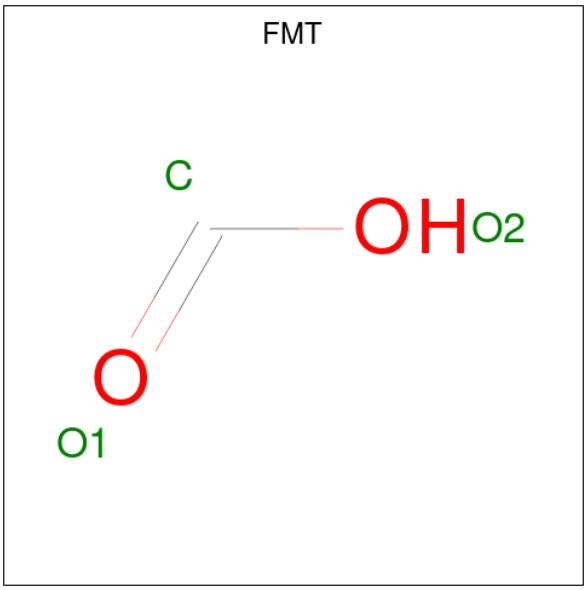
Chain	Residue	Modelled	Actual	Comment	Reference
C	138	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
C	146	GLY	-	CLONING ARTIFACT	UNP Q9XA42
C	147	SER	-	CLONING ARTIFACT	UNP Q9XA42
D	-1	GLY	-	CLONING ARTIFACT	UNP Q9XA42
D	0	HIS	-	CLONING ARTIFACT	UNP Q9XA42
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
D	26	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
D	68	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
D	138	MSE	MET	MODIFIED RESIDUE	UNP Q9XA42
D	146	GLY	-	CLONING ARTIFACT	UNP Q9XA42
D	147	SER	-	CLONING ARTIFACT	UNP Q9XA42

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 1 2	0	0
2	C	1	Total C O 3 1 2	0	0
2	D	1	Total C O 3 1 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	57	Total O 57 57	0	0

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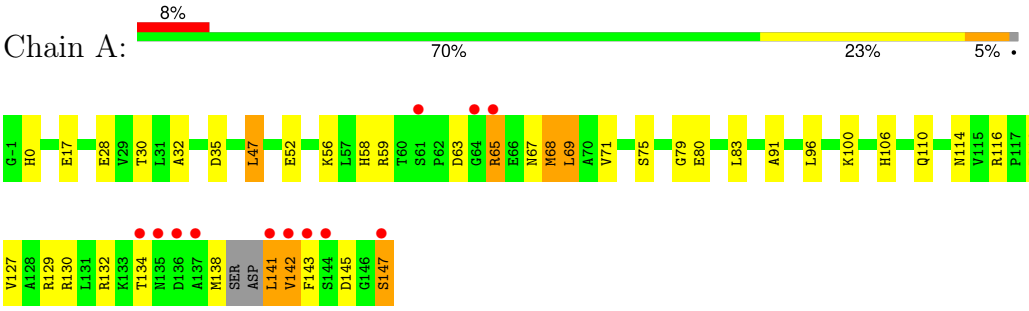
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	59	Total O 59 59	0	0
3	C	70	Total O 70 70	0	0
3	D	65	Total O 65 65	0	0

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.

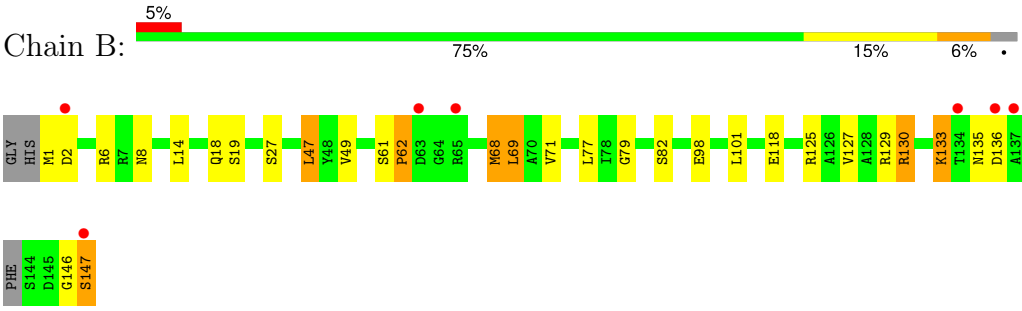
• Molecule 1: Putative transcriptional regulator

Chain A:



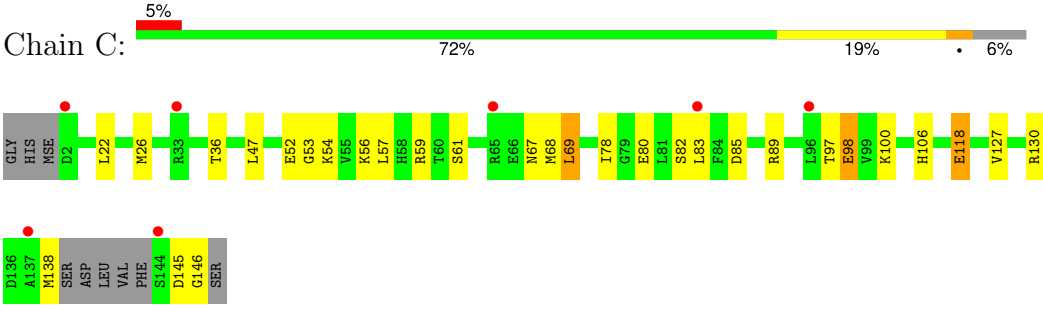
• Molecule 1: Putative transcriptional regulator

Chain B:



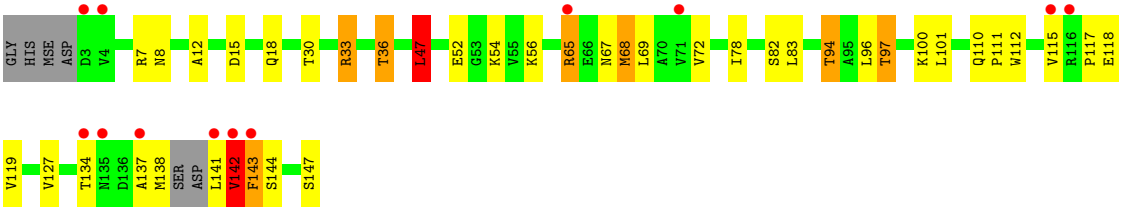
• Molecule 1: Putative transcriptional regulator

Chain C:



• Molecule 1: Putative transcriptional regulator

Chain D:


GLY
HIS
MSE
ASP
D3
V4
R7
N8
A12
D15
Q18
T30
R33
T36
L47
E52
G53
K54
V55
K56
R65
E66
N67
M68
L69
A70
V71
V72
I78
S82
L83
T94
A95
L96
T97
K100
L101
Q110
P111
W112
V115
R116
P117
E118
V119
V127
T134
N135
D136
A137
M138
SER
ASP
L141
V142
F143
S144
S147

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	39.85Å 100.95Å 144.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.94 – 2.00 33.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.94-2.00) 99.4 (33.93-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.281 0.228 , 0.277	Depositor DCC
R_{free} test set	2012 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.7	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	0.94	EDS
Total number of atoms	4667	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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

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

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	0.58	0/1146	0.69	0/1543
1	B	0.56	0/1119	0.76	1/1508 (0.1%)
1	C	0.62	0/1079	0.77	0/1457
1	D	0.52	0/1125	0.75	2/1517 (0.1%)
All	All	0.57	0/4469	0.74	3/6025 (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
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	47	LEU	CA-CB-CG	8.07	133.87	115.30
1	D	47	LEU	CB-CG-CD2	5.86	120.96	111.00
1	B	47	LEU	CA-CB-CG	5.83	128.71	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	SER	Peptide

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Mol	Chain	Res	Type	Group
1	D	142	VAL	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	1130	0	1138	43	0
1	B	1104	0	1108	34	0
1	C	1067	0	1069	32	0
1	D	1106	0	1118	50	0
2	A	3	0	1	0	0
2	C	3	0	1	0	0
2	D	3	0	1	0	0
3	A	57	0	0	2	0
3	B	59	0	0	1	0
3	C	70	0	0	3	0
3	D	65	0	0	3	0
All	All	4667	0	4436	123	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 (123) 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:56:LYS:HG3	1:D:68:MSE:CE	1.87	1.04
1:B:69:LEU:C	1:B:69:LEU:HD23	1.77	1.04
1:A:110:GLN:OE1	1:D:117:PRO:HB2	1.59	1.02
1:D:56:LYS:HG3	1:D:68:MSE:HE1	1.35	1.01
1:B:69:LEU:HD23	1:B:69:LEU:O	1.67	0.94
1:A:134:THR:HG21	1:D:134:THR:HB	1.46	0.93
1:D:33[A]:ARG:NH1	1:D:97:THR:HA	1.86	0.89
1:D:54:LYS:H	1:D:97:THR:CG2	1.86	0.88
1:D:94:THR:HB	3:D:309:HOH:O	1.72	0.87
1:B:138:MSE:HE1	1:D:141:LEU:CD1	2.05	0.86
1:A:116:ARG:HD3	3:A:356:HOH:O	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:HD21	1:D:144:SER:HB3	1.61	0.81
1:B:61:SER:OG	1:B:62:PRO:HD2	1.81	0.80
1:A:68:MSE:HE2	1:A:71:VAL:HG23	1.62	0.79
1:B:69:LEU:C	1:B:69:LEU:CD2	2.50	0.78
1:A:142:VAL:HG13	1:A:143:PHE:H	1.48	0.78
1:C:134:THR:HG22	1:C:135:ASN:N	2.00	0.76
1:A:141:LEU:CD1	1:C:138:MSE:HE1	2.16	0.75
1:B:79:GLY:HA2	1:D:147:SER:HA	1.69	0.74
1:B:138:MSE:HE1	1:D:141:LEU:HD11	1.67	0.74
1:B:49:VAL:HG22	1:B:77:LEU:HD22	1.70	0.72
1:D:56:LYS:HG3	1:D:68:MSE:HE3	1.72	0.72
1:C:54:LYS:H	1:C:97:THR:HG22	1.54	0.71
1:D:54:LYS:H	1:D:97:THR:HG21	1.54	0.71
1:A:141:LEU:HD12	1:C:138:MSE:HE1	1.72	0.70
1:C:54:LYS:H	1:C:97:THR:CG2	2.04	0.69
1:B:69:LEU:HD21	1:D:144:SER:CB	2.23	0.69
1:B:138:MSE:HE1	1:D:141:LEU:HD12	1.74	0.68
1:C:130:ARG:HD2	3:C:351:HOH:O	1.93	0.68
1:B:130:ARG:HD3	1:D:143:PHE:HZ	1.61	0.66
1:B:69:LEU:CD2	1:D:144:SER:HB3	2.26	0.66
1:C:138:MSE:HG2	1:D:138:MSE:HE2	1.77	0.65
1:A:141:LEU:HD12	1:C:138:MSE:CE	2.27	0.64
1:A:147:SER:HA	1:C:89:ARG:HH11	1.64	0.63
1:C:134:THR:CG2	1:C:135:ASN:N	2.62	0.63
1:A:127:VAL:HG12	1:D:127:VAL:HG12	1.80	0.62
1:C:97:THR:HG23	1:C:98:GLU:O	2.00	0.62
1:D:33[A]:ARG:CZ	1:D:96:LEU:O	2.48	0.62
1:B:130:ARG:HD3	1:D:143:PHE:CZ	2.34	0.61
1:D:33[A]:ARG:HH12	1:D:97:THR:HA	1.63	0.61
1:A:138:MSE:HG3	1:C:138:MSE:HE2	1.82	0.60
1:A:83:LEU:O	1:A:106:HIS:HD2	1.84	0.60
1:A:134:THR:O	1:A:138:MSE:HB3	2.01	0.60
1:D:54:LYS:N	1:D:97:THR:HG21	2.16	0.60
1:C:52:GLU:HG2	1:C:100:LYS:HB2	1.84	0.59
1:D:56:LYS:CG	1:D:68:MSE:HE1	2.23	0.59
1:D:47:LEU:HD13	1:D:83:LEU:HD22	1.85	0.58
1:A:134:THR:O	1:A:138:MSE:HE3	2.04	0.58
1:A:141:LEU:HD13	1:B:138:MSE:SE	2.54	0.58
1:A:80:GLU:OE2	1:A:130:ARG:NH1	2.20	0.57
1:A:121:THR:HG21	3:D:353:HOH:O	2.03	0.57
1:C:118:GLU:O	1:C:118:GLU:CD	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HD2	1:C:85:ASP:OD2	2.05	0.56
1:C:61:SER:OG	1:C:67:ASN:HB2	2.07	0.55
1:D:142:VAL:HG13	1:D:143:PHE:N	2.22	0.54
1:A:134:THR:HG21	1:D:134:THR:CB	2.31	0.54
1:D:36:THR:HG23	3:D:324:HOH:O	2.08	0.54
1:A:68:MSE:HE3	1:B:68:MSE:SE	2.58	0.53
1:A:52:GLU:HG2	1:A:100:LYS:HB2	1.91	0.52
1:D:67:ASN:HD21	1:D:69:LEU:HD21	1.73	0.52
1:A:118:GLU:HG3	3:A:356:HOH:O	2.10	0.52
1:C:53:GLY:CA	1:C:97:THR:HG21	2.40	0.52
1:A:91:ALA:HB3	1:C:146:GLY:HA2	1.92	0.51
1:D:142:VAL:CG1	1:D:143:PHE:N	2.73	0.51
1:B:14:LEU:HB3	1:B:18:GLN:HG3	1.91	0.51
1:A:134:THR:HG23	1:D:138:MSE:SE	2.61	0.51
1:D:67:ASN:ND2	1:D:69:LEU:HD21	2.25	0.50
1:B:8:ASN:ND2	1:B:77:LEU:HD21	2.26	0.50
1:A:143:PHE:HE2	1:C:80:GLU:OE1	1.95	0.50
1:D:137:ALA:O	1:D:141:LEU:N	2.45	0.50
1:C:59:ARG:HE	1:C:69:LEU:HD21	1.78	0.49
1:C:53:GLY:HA2	1:C:97:THR:HG21	1.94	0.49
1:B:69:LEU:HD21	1:D:144:SER:CA	2.43	0.49
1:D:110:GLN:HB3	1:D:111:PRO:HD3	1.95	0.48
1:A:59:ARG:CZ	1:A:69:LEU:HD11	2.44	0.47
1:A:147:SER:HB3	1:C:82:SER:HB3	1.95	0.47
1:A:56:LYS:HB2	1:A:96:LEU:HD11	1.96	0.47
1:D:52:GLU:HG2	1:D:100:LYS:HB2	1.96	0.47
1:B:146:GLY:O	1:B:147:SER:HB2	2.14	0.47
1:B:129:ARG:CZ	3:C:363:HOH:O	2.62	0.47
1:D:112:TRP:CZ2	1:D:119:VAL:HG11	2.50	0.47
1:D:134:THR:O	1:D:138:MSE:HB3	2.14	0.47
1:B:79:GLY:O	1:B:82:SER:HB3	2.15	0.47
1:C:83:LEU:O	1:C:106:HIS:HD2	1.97	0.47
1:D:8:ASN:O	1:D:12:ALA:HB2	2.14	0.47
1:A:47:LEU:C	1:A:47:LEU:HD23	2.36	0.46
1:D:65:ARG:HD3	1:D:65:ARG:HA	1.79	0.45
1:A:145:ASP:HB2	1:C:78:ILE:HA	1.97	0.45
1:B:127:VAL:HG12	1:C:127:VAL:HG12	1.99	0.45
1:A:145:ASP:HA	1:C:57:LEU:CD1	2.48	0.44
1:B:130:ARG:HE	1:B:130:ARG:HB3	1.43	0.44
1:D:33[A]:ARG:NH2	1:D:96:LEU:O	2.50	0.44
1:A:56:LYS:HE3	1:A:58:HIS:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ARG:NH2	3:B:161:HOH:O	2.45	0.44
1:A:47:LEU:HD13	1:A:83:LEU:HD22	1.99	0.43
1:B:129:ARG:HG3	1:B:133:LYS:HD3	1.98	0.43
1:A:116:ARG:HG3	1:A:119:VAL:HG23	2.01	0.43
1:D:115:VAL:O	1:D:117:PRO:HD3	2.19	0.43
1:A:79:GLY:H	1:C:145:ASP:HB3	1.84	0.43
1:A:65:ARG:NH1	1:A:67:ASN:OD1	2.51	0.43
1:A:114:ASN:HD22	1:A:114:ASN:N	2.17	0.43
1:C:22:LEU:O	1:C:26:MSE:HG3	2.18	0.43
1:B:68:MSE:HE1	1:B:71:VAL:HG23	2.01	0.42
1:D:33[A]:ARG:HH11	1:D:33[A]:ARG:HB2	1.84	0.42
1:D:72:VAL:HG11	1:D:78:ILE:HG13	2.01	0.42
1:B:133:LYS:HA	1:B:136:ASP:HB2	2.01	0.42
1:A:138:MSE:HE2	1:D:138:MSE:HE3	2.00	0.42
1:A:142:VAL:HG13	1:A:143:PHE:N	2.26	0.42
1:A:83:LEU:O	1:A:106:HIS:CD2	2.69	0.41
1:A:134:THR:HG23	1:D:138:MSE:CE	2.49	0.41
1:A:141:LEU:CD1	1:B:138:MSE:SE	3.18	0.41
1:B:49:VAL:HG22	1:B:77:LEU:CD2	2.46	0.41
1:A:143:PHE:HB2	1:B:135:ASN:ND2	2.35	0.41
1:B:138:MSE:HB3	1:B:139:SER:H	1.68	0.41
1:C:134:THR:HG21	1:D:141:LEU:HD21	2.00	0.41
1:D:138:MSE:HA	1:D:141:LEU:HD13	2.02	0.41
1:B:1:MSE:HE3	1:B:6:ARG:HB3	2.02	0.41
1:C:56:LYS:HE2	1:C:68:MSE:HB2	2.03	0.41
1:D:15:ASP:OD1	1:D:18:GLN:HG3	2.21	0.40
1:A:32:ALA:O	1:A:35:ASP:HB2	2.21	0.40
1:C:59:ARG:HE	1:C:59:ARG:HB2	1.77	0.40
1:C:135:ASN:HB3	3:C:362:HOH:O	2.21	0.40
1:D:54:LYS:H	1:D:97:THR:HG23	1.78	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	144/149 (97%)	138 (96%)	5 (4%)	1 (1%)	22 16
1	B	141/149 (95%)	136 (96%)	3 (2%)	2 (1%)	11 5
1	C	136/149 (91%)	130 (96%)	6 (4%)	0	100 100
1	D	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	22 16
All	All	562/596 (94%)	540 (96%)	18 (3%)	4 (1%)	22 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	143	PHE
1	A	142	VAL
1	B	138	MSE
1	B	62	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	121/118 (102%)	107 (88%)	14 (12%)	5 3
1	B	119/118 (101%)	107 (90%)	12 (10%)	7 4
1	C	114/118 (97%)	107 (94%)	7 (6%)	18 14
1	D	119/118 (101%)	105 (88%)	14 (12%)	5 3
All	All	473/472 (100%)	426 (90%)	47 (10%)	8 4

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	17	GLU
1	A	28	GLU
1	A	30	THR

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Mol	Chain	Res	Type
1	A	47	LEU
1	A	63	ASP
1	A	65	ARG
1	A	68	MSE
1	A	69	LEU
1	A	75	SER
1	A	129	ARG
1	A	132	ARG
1	A	141	LEU
1	A	147	SER
1	B	2	ASP
1	B	19	SER
1	B	27	SER
1	B	47	LEU
1	B	68	MSE
1	B	69	LEU
1	B	98	GLU
1	B	101	LEU
1	B	118	GLU
1	B	130	ARG
1	B	133	LYS
1	B	147	SER
1	C	36	THR
1	C	47	LEU
1	C	69	LEU
1	C	98	GLU
1	C	118	GLU
1	C	133	LYS
1	C	134	THR
1	D	7	ARG
1	D	30	THR
1	D	33[A]	ARG
1	D	33[B]	ARG
1	D	36	THR
1	D	47	LEU
1	D	65	ARG
1	D	68	MSE
1	D	82	SER
1	D	94	THR
1	D	97	THR
1	D	101	LEU
1	D	118	GLU

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Mol	Chain	Res	Type
1	D	142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	110	GLN
1	A	114	ASN
1	A	135	ASN
1	B	135	ASN
1	C	106	HIS
1	C	135	ASN
1	D	67	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 ligands 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	FMT	C	302	-	2,2,2	0.76	0	1,1,1	0.46	0
2	FMT	A	301	-	2,2,2	0.73	0	1,1,1	0.28	0
2	FMT	D	303	-	2,2,2	0.65	0	1,1,1	0.35	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	143/149 (95%)	0.58	12 (8%) 11 10	31, 38, 56, 64	0
1	B	140/149 (93%)	0.52	8 (5%) 23 23	25, 37, 55, 58	0
1	C	137/149 (91%)	0.59	8 (5%) 23 22	30, 39, 51, 71	0
1	D	140/149 (93%)	0.56	12 (8%) 10 9	30, 37, 55, 59	0
All	All	560/596 (93%)	0.56	40 (7%) 16 15	25, 38, 55, 71	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	THR	8.0
1	A	141	LEU	7.1
1	A	143	PHE	6.1
1	A	65	ARG	4.8
1	D	135	ASN	4.1
1	A	134	THR	3.9
1	D	115	VAL	3.8
1	D	137	ALA	3.7
1	A	135	ASN	3.7
1	C	2	ASP	3.5
1	A	136	ASP	3.4
1	C	134	THR	3.3
1	D	71	VAL	3.3
1	C	96	LEU	3.3
1	A	61	SER	3.2
1	A	64	GLY	3.2
1	D	142	VAL	3.2
1	C	137	ALA	3.1
1	B	2	ASP	3.0
1	B	134	THR	3.0
1	B	147	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	141	LEU	2.8
1	D	143	PHE	2.7
1	A	137	ALA	2.7
1	B	137	ALA	2.6
1	C	144	SER	2.6
1	C	83	LEU	2.5
1	A	142	VAL	2.5
1	B	63	ASP	2.4
1	A	144	SER	2.4
1	D	4	VAL	2.4
1	C	65	ARG	2.4
1	D	3	ASP	2.4
1	A	147	SER	2.3
1	D	65	ARG	2.3
1	B	140	ASP	2.3
1	B	136	ASP	2.3
1	C	33	ARG	2.2
1	D	116	ARG	2.0
1	B	65	ARG	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)

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, 95^{th} 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	FMT	C	302	3/3	0.66	0.26	37,37,37,38	0
2	FMT	A	301	3/3	0.80	0.13	76,76,76,76	0
2	FMT	D	303	3/3	0.90	0.32	35,35,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.