Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:06 am BST

PDB ID	:	1XM3
Title	:	Crystal structure of Northeast Structural Genomics Target SR156
Authors	:	Kuzin, A.; Abashidze, M.; Vorobiev, S.; Forouhar, F.; Acton, T.; Ma, L.; Xiao, R.; Montelione, G.; Tong, L.; Hunt, J.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2004-10-01
Resolution	:	1.80 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 ⓘ symbol.

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

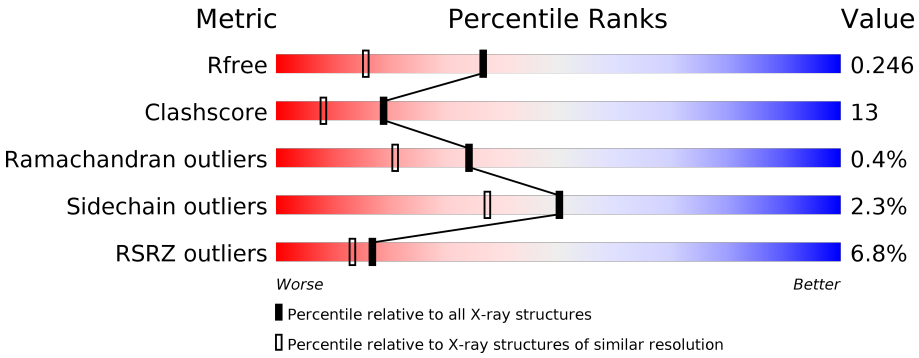
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	6% 72% 19% • 8%
1	B	264	9% 73% 21% • 5%
1	C	264	5% 69% 25% • 6%
1	D	264	5% 71% 21% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7985 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 Thiazole biosynthesis protein thiG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	Se	0	0	0
			1804	1143	301	351	2	7			
1	B	251	Total	C	N	O	S	Se	0	0	0
			1859	1177	310	363	2	7			
1	C	249	Total	C	N	O	S	Se	0	0	0
			1846	1170	308	359	2	7			
1	D	249	Total	C	N	O	S	Se	0	0	0
			1846	1170	308	359	2	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MSE	MET	MODIFIED RESIDUE	UNP O31618
A	47	MSE	MET	MODIFIED RESIDUE	UNP O31618
A	96	MSE	MET	MODIFIED RESIDUE	UNP O31618
A	152	MSE	MET	MODIFIED RESIDUE	UNP O31618
A	197	MSE	MET	MODIFIED RESIDUE	UNP O31618
A	219	MSE	MET	MODIFIED RESIDUE	UNP O31618
A	223	MSE	MET	MODIFIED RESIDUE	UNP O31618
A	257	LEU	-	CLONING ARTIFACT	UNP O31618
A	258	GLU	-	CLONING ARTIFACT	UNP O31618
A	259	HIS	-	EXPRESSION TAG	UNP O31618
A	259	HIS	-	EXPRESSION TAG	UNP O31618
A	260	HIS	-	EXPRESSION TAG	UNP O31618
A	261	HIS	-	EXPRESSION TAG	UNP O31618
A	262	HIS	-	EXPRESSION TAG	UNP O31618
A	263	HIS	-	EXPRESSION TAG	UNP O31618
B	3	MSE	MET	MODIFIED RESIDUE	UNP O31618
B	47	MSE	MET	MODIFIED RESIDUE	UNP O31618
B	96	MSE	MET	MODIFIED RESIDUE	UNP O31618
B	152	MSE	MET	MODIFIED RESIDUE	UNP O31618
B	197	MSE	MET	MODIFIED RESIDUE	UNP O31618
B	219	MSE	MET	MODIFIED RESIDUE	UNP O31618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	223	MSE	MET	MODIFIED RESIDUE	UNP O31618
B	257	LEU	-	CLONING ARTIFACT	UNP O31618
B	258	GLU	-	CLONING ARTIFACT	UNP O31618
B	259	HIS	-	EXPRESSION TAG	UNP O31618
B	259	HIS	-	EXPRESSION TAG	UNP O31618
B	260	HIS	-	EXPRESSION TAG	UNP O31618
B	261	HIS	-	EXPRESSION TAG	UNP O31618
B	262	HIS	-	EXPRESSION TAG	UNP O31618
B	263	HIS	-	EXPRESSION TAG	UNP O31618
C	3	MSE	MET	MODIFIED RESIDUE	UNP O31618
C	47	MSE	MET	MODIFIED RESIDUE	UNP O31618
C	96	MSE	MET	MODIFIED RESIDUE	UNP O31618
C	152	MSE	MET	MODIFIED RESIDUE	UNP O31618
C	197	MSE	MET	MODIFIED RESIDUE	UNP O31618
C	219	MSE	MET	MODIFIED RESIDUE	UNP O31618
C	223	MSE	MET	MODIFIED RESIDUE	UNP O31618
C	257	LEU	-	CLONING ARTIFACT	UNP O31618
C	258	GLU	-	CLONING ARTIFACT	UNP O31618
C	259	HIS	-	EXPRESSION TAG	UNP O31618
C	259	HIS	-	EXPRESSION TAG	UNP O31618
C	260	HIS	-	EXPRESSION TAG	UNP O31618
C	261	HIS	-	EXPRESSION TAG	UNP O31618
C	262	HIS	-	EXPRESSION TAG	UNP O31618
C	263	HIS	-	EXPRESSION TAG	UNP O31618
D	3	MSE	MET	MODIFIED RESIDUE	UNP O31618
D	47	MSE	MET	MODIFIED RESIDUE	UNP O31618
D	96	MSE	MET	MODIFIED RESIDUE	UNP O31618
D	152	MSE	MET	MODIFIED RESIDUE	UNP O31618
D	197	MSE	MET	MODIFIED RESIDUE	UNP O31618
D	219	MSE	MET	MODIFIED RESIDUE	UNP O31618
D	223	MSE	MET	MODIFIED RESIDUE	UNP O31618
D	257	LEU	-	CLONING ARTIFACT	UNP O31618
D	258	GLU	-	CLONING ARTIFACT	UNP O31618
D	259	HIS	-	EXPRESSION TAG	UNP O31618
D	259	HIS	-	EXPRESSION TAG	UNP O31618
D	260	HIS	-	EXPRESSION TAG	UNP O31618
D	261	HIS	-	EXPRESSION TAG	UNP O31618
D	262	HIS	-	EXPRESSION TAG	UNP O31618
D	263	HIS	-	EXPRESSION TAG	UNP O31618

- Molecule 2 is water.

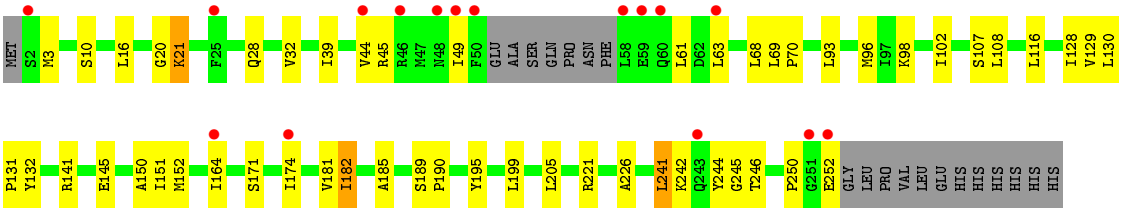
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	153	Total O 153 153	0	0
2	B	163	Total O 163 163	0	0
2	C	146	Total O 146 146	0	0
2	D	168	Total O 168 168	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

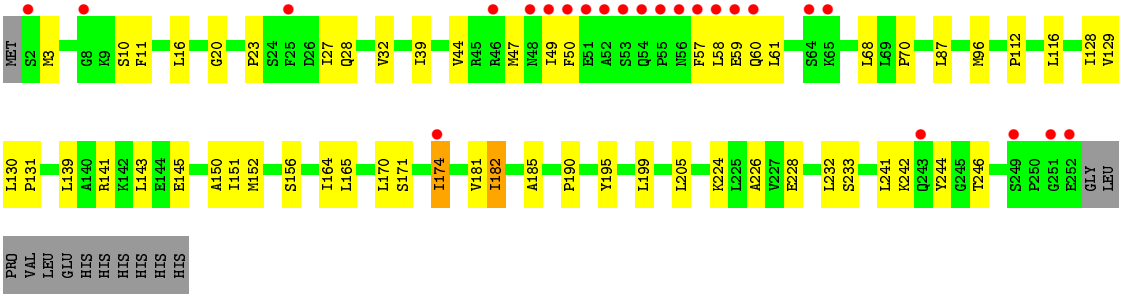
- Molecule 1: Thiazole biosynthesis protein thiG

Chain A:



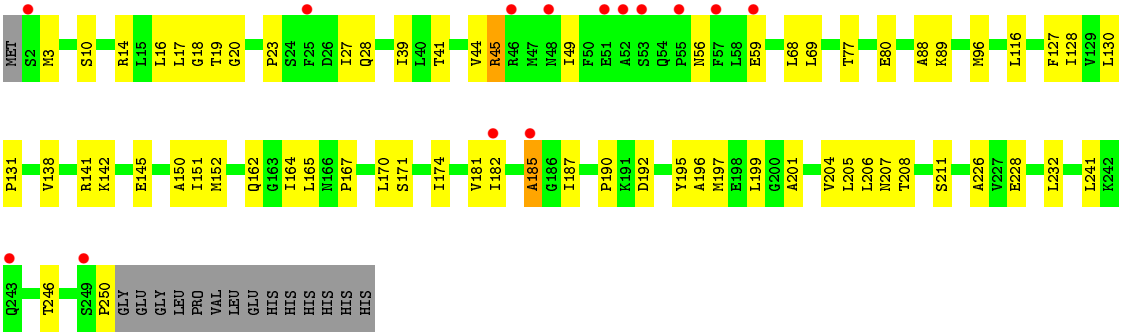
- Molecule 1: Thiazole biosynthesis protein thiG

Chain B:



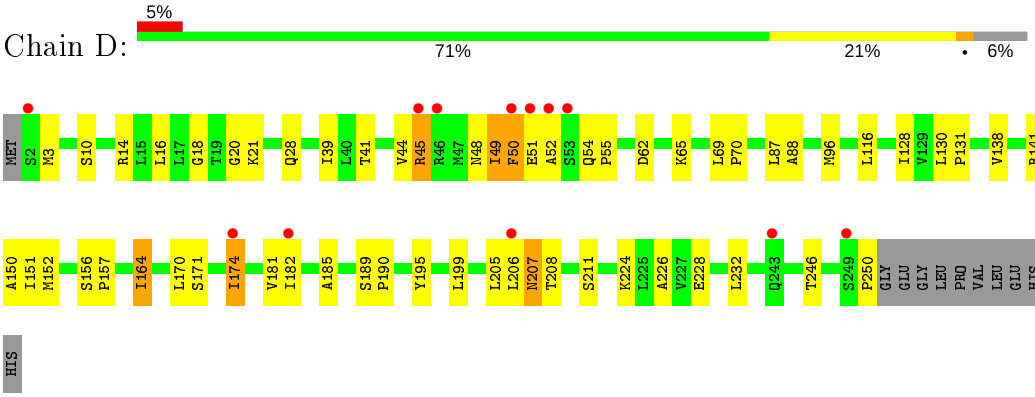
- Molecule 1: Thiazole biosynthesis protein thiG

Chain C:



• Molecule 1: Thiazole biosynthesis protein thiG

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.54Å 120.72Å 74.24Å 90.00° 108.32° 90.00°	Depositor
Resolution (Å)	29.82 – 1.80 29.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (29.82-1.80) 98.2 (29.82-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.237 0.224 , 0.246	Depositor DCC
R_{free} test set	10625 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7985	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.39% 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	0.29	0/1821	0.58	1/2452 (0.0%)
1	B	0.30	0/1879	0.57	1/2533 (0.0%)
1	C	0.29	0/1866	0.59	1/2516 (0.0%)
1	D	0.30	0/1866	0.60	1/2516 (0.0%)
All	All	0.30	0/7432	0.58	4/10017 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	128	ILE	N-CA-C	-5.65	95.74	111.00
1	A	128	ILE	N-CA-C	-5.55	96.02	111.00
1	C	128	ILE	N-CA-C	-5.26	96.80	111.00
1	B	128	ILE	N-CA-C	-5.22	96.92	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1804	0	1861	47	0
1	B	1859	0	1908	47	0
1	C	1846	0	1899	59	0
1	D	1846	0	1899	50	0
2	A	153	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	163	0	0	1	0
2	C	146	0	0	4	0
2	D	168	0	0	5	0
All	All	7985	0	7567	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 13.

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:197:MSE:HE3	1:C:204:VAL:HG23	1.51	0.91
1:B:182:ILE:HD11	1:B:205:LEU:HB2	1.55	0.86
1:C:164:ILE:HD11	1:C:167:PRO:HA	1.58	0.85
1:D:62:ASP:HB3	1:D:65:LYS:HE2	1.59	0.84
1:A:250:PRO:HG2	1:C:241:LEU:HD13	1.62	0.81
1:B:58:LEU:HA	1:B:61:LEU:HD12	1.63	0.80
1:B:59:GLU:HG3	1:B:60:GLN:HG3	1.64	0.79
1:C:182:ILE:HD11	1:C:205:LEU:HB2	1.63	0.79
1:D:207:ASN:HD22	1:D:208:THR:H	1.31	0.78
1:A:182:ILE:HD11	1:A:205:LEU:HB2	1.66	0.77
1:C:3:MSE:HE2	1:C:10:SER:HB3	1.66	0.77
1:C:171:SER:HA	1:C:174:ILE:HD11	1.66	0.76
1:C:197:MSE:HE3	1:C:204:VAL:CG2	2.16	0.75
1:A:171:SER:HA	1:A:174:ILE:HD11	1.68	0.75
1:B:171:SER:HA	1:B:174:ILE:HD11	1.69	0.74
1:C:20:GLY:H	1:C:28:GLN:NE2	1.85	0.74
1:B:152:MSE:HG2	1:B:182:ILE:HG23	1.71	0.72
1:C:174:ILE:HD12	1:C:199:LEU:O	1.90	0.71
1:D:182:ILE:HD11	1:D:205:LEU:HB2	1.71	0.71
1:C:197:MSE:CE	1:C:201:ALA:HB3	2.21	0.71
1:C:197:MSE:CE	1:C:204:VAL:HG23	2.20	0.71
1:D:51:GLU:HG2	1:D:52:ALA:H	1.54	0.71
1:A:174:ILE:HD12	1:A:199:LEU:O	1.91	0.69
1:B:174:ILE:HD12	1:B:199:LEU:O	1.92	0.69
1:A:164:ILE:HD11	1:A:195:TYR:CE2	2.28	0.68
1:A:151:ILE:HD11	1:A:181:VAL:HG22	1.75	0.67
1:D:20:GLY:H	1:D:28:GLN:NE2	1.92	0.66
1:A:171:SER:HB3	1:C:246:THR:HB	1.79	0.65
1:C:16:LEU:HD13	1:C:182:ILE:HD12	1.79	0.65
1:B:112:PRO:O	1:B:116:LEU:HD13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:MSE:HE2	1:C:201:ALA:HB3	1.78	0.64
1:B:171:SER:HB3	1:D:246:THR:HB	1.78	0.64
1:A:3:MSE:HE2	1:A:10:SER:HB3	1.79	0.64
1:A:63:LEU:HD12	1:A:63:LEU:H	1.64	0.63
1:A:16:LEU:HD13	1:A:182:ILE:HD12	1.79	0.63
1:B:16:LEU:HD22	1:B:182:ILE:CD1	2.28	0.63
1:B:164:ILE:HG22	2:B:284:HOH:O	1.98	0.62
1:D:171:SER:HA	1:D:174:ILE:HD11	1.80	0.62
1:A:164:ILE:HG13	1:A:164:ILE:O	1.99	0.62
1:D:151:ILE:HD11	1:D:181:VAL:HG22	1.82	0.62
1:D:16:LEU:HD13	1:D:182:ILE:HD12	1.83	0.61
1:B:47:MSE:HE3	1:B:57:PHE:H	1.66	0.60
1:B:151:ILE:HD11	1:B:181:VAL:HG22	1.82	0.60
1:C:131:PRO:HD2	1:C:150:ALA:O	2.01	0.60
1:A:16:LEU:HD22	1:A:182:ILE:CD1	2.32	0.59
1:A:98:LYS:NZ	1:A:132:TYR:HB2	2.17	0.59
1:B:116:LEU:HD12	1:B:143:LEU:HD21	1.83	0.59
1:C:228:GLU:O	1:C:232:LEU:HD13	2.02	0.59
1:D:174:ILE:HD12	1:D:199:LEU:O	2.02	0.59
1:A:246:THR:HB	1:C:171:SER:HB3	1.85	0.59
1:C:151:ILE:HD11	1:C:181:VAL:HG22	1.85	0.58
1:C:16:LEU:HD22	1:C:182:ILE:CD1	2.33	0.58
1:D:20:GLY:H	1:D:28:GLN:HE22	1.51	0.58
1:B:246:THR:HB	1:D:171:SER:HB3	1.85	0.58
1:A:152:MSE:HG2	1:A:182:ILE:HG23	1.86	0.58
1:D:228:GLU:O	1:D:232:LEU:HD13	2.03	0.58
1:B:47:MSE:HE3	1:B:57:PHE:N	2.18	0.57
1:C:162:GLN:HE21	1:C:165:LEU:HD21	1.68	0.57
1:B:16:LEU:HD13	1:B:182:ILE:HD12	1.84	0.57
1:B:49:ILE:HG13	1:B:50:PHE:HD1	1.68	0.57
1:B:116:LEU:HD11	1:B:139:LEU:HD11	1.87	0.57
1:A:131:PRO:HD2	1:A:150:ALA:O	2.05	0.57
1:A:171:SER:HA	1:A:174:ILE:CD1	2.33	0.56
1:C:56:ASN:HD22	1:C:59:GLU:HG2	1.69	0.56
1:B:131:PRO:HD2	1:B:150:ALA:O	2.05	0.56
1:D:69:LEU:HD13	1:D:96:MSE:HE3	1.87	0.56
1:D:3:MSE:HE2	1:D:10:SER:HB3	1.86	0.56
1:D:207:ASN:ND2	1:D:208:THR:H	2.02	0.56
1:C:171:SER:HA	1:C:174:ILE:CD1	2.35	0.55
1:B:50:PHE:CZ	1:B:87:LEU:HD23	2.41	0.55
1:D:16:LEU:HD22	1:D:182:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LEU:HD13	1:C:96:MSE:HE3	1.88	0.55
1:C:68:LEU:N	1:C:68:LEU:HD22	2.23	0.54
1:A:98:LYS:HZ2	1:A:132:TYR:HB2	1.72	0.54
1:D:44:VAL:HG13	1:D:49:ILE:HD11	1.89	0.53
1:D:45:ARG:HA	1:D:50:PHE:HE2	1.74	0.53
1:D:164:ILE:HG21	1:D:195:TYR:CD2	2.43	0.53
1:D:131:PRO:HD2	1:D:150:ALA:O	2.08	0.53
1:B:190:PRO:HB3	1:B:226:ALA:HB2	1.91	0.52
1:C:23:PRO:HB2	1:C:27:ILE:HD12	1.91	0.52
1:C:197:MSE:HE1	1:C:201:ALA:HB3	1.92	0.52
1:A:28:GLN:O	1:A:32:VAL:HG23	2.10	0.51
1:C:20:GLY:H	1:C:28:GLN:HE22	1.58	0.51
1:C:56:ASN:O	1:C:59:GLU:HG3	2.10	0.51
1:A:141:ARG:O	1:A:145:GLU:HG3	2.11	0.51
1:B:3:MSE:HE2	1:B:10:SER:HB3	1.92	0.51
1:C:152:MSE:HG2	1:C:182:ILE:HG23	1.91	0.51
1:D:138:VAL:O	1:D:142:LYS:HG2	2.10	0.51
1:C:164:ILE:HG22	2:C:282:HOH:O	2.10	0.51
1:B:171:SER:HA	1:B:174:ILE:CD1	2.39	0.50
1:B:50:PHE:CE2	1:B:87:LEU:HD23	2.45	0.50
1:B:228:GLU:O	1:B:232:LEU:HD13	2.12	0.50
1:C:89:LYS:HD2	1:C:127:PHE:CZ	2.47	0.50
1:A:70:PRO:HD2	1:A:96:MSE:O	2.11	0.50
1:A:45:ARG:HB3	1:A:45:ARG:NH1	2.27	0.50
1:A:190:PRO:HB3	1:A:226:ALA:HB2	1.94	0.50
1:B:164:ILE:HG21	1:B:195:TYR:CD2	2.47	0.50
1:C:14:ARG:NH2	2:C:314:HOH:O	2.44	0.49
1:D:16:LEU:HG	1:D:39:ILE:HB	1.94	0.49
1:D:45:ARG:HA	1:D:50:PHE:CE2	2.47	0.49
1:D:44:VAL:HG21	1:D:88:ALA:HB2	1.94	0.49
1:C:18:GLY:HA2	1:C:41:THR:HG22	1.94	0.49
1:B:224:LYS:O	1:B:228:GLU:HG3	2.13	0.49
1:A:44:VAL:CG2	1:A:70:PRO:HB2	2.43	0.48
1:C:190:PRO:HB3	1:C:226:ALA:HB2	1.94	0.48
1:A:241:LEU:HD22	1:C:250:PRO:O	2.14	0.48
1:C:182:ILE:CD1	1:C:205:LEU:HB2	2.41	0.48
1:D:164:ILE:HD13	1:D:170:LEU:HD22	1.95	0.48
1:C:164:ILE:HG21	1:C:195:TYR:CD2	2.48	0.48
1:A:221:ARG:HH11	1:A:221:ARG:HG2	1.78	0.48
1:C:44:VAL:HG13	1:C:49:ILE:HD11	1.95	0.48
1:D:70:PRO:HD2	1:D:96:MSE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:PRO:HB3	1:D:226:ALA:HB2	1.96	0.48
1:D:54:GLN:HB3	1:D:55:PRO:HD2	1.95	0.48
1:B:20:GLY:H	1:B:28:GLN:NE2	2.12	0.47
1:C:141:ARG:O	1:C:145:GLU:HG3	2.13	0.47
1:C:208:THR:HA	1:C:211:SER:OG	2.13	0.47
1:D:224:LYS:O	1:D:228:GLU:HG3	2.14	0.47
1:D:141:ARG:O	1:D:145:GLU:HG3	2.15	0.47
1:B:28:GLN:O	1:B:32:VAL:HG23	2.15	0.47
1:C:197:MSE:HE2	1:C:197:MSE:N	2.29	0.47
1:B:23:PRO:HG2	1:B:27:ILE:HD12	1.96	0.47
1:D:164:ILE:HG22	2:D:285:HOH:O	2.14	0.47
1:A:49:ILE:HD13	1:A:93:LEU:HD12	1.97	0.47
1:B:3:MSE:HE3	1:B:11:PHE:C	2.35	0.46
1:A:68:LEU:HD22	1:A:68:LEU:N	2.31	0.46
1:C:45:ARG:O	1:C:45:ARG:HD3	2.14	0.46
1:D:130:LEU:HG	1:D:150:ALA:HB3	1.96	0.46
1:C:205:LEU:C	1:C:205:LEU:HD23	2.36	0.46
1:B:242:LYS:HD3	1:B:244:TYR:CZ	2.51	0.46
1:C:185:ALA:HB3	2:C:310:HOH:O	2.16	0.46
1:D:14:ARG:NH2	2:D:406:HOH:O	2.44	0.46
1:A:242:LYS:HD3	1:A:244:TYR:CZ	2.51	0.46
1:D:164:ILE:HD12	2:D:286:HOH:O	2.15	0.46
1:A:69:LEU:HD13	1:A:96:MSE:HE3	1.98	0.45
1:C:196:ALA:C	1:C:197:MSE:HE2	2.36	0.45
1:D:208:THR:HA	1:D:211:SER:OG	2.17	0.45
1:D:130:LEU:HD12	1:D:130:LEU:N	2.31	0.45
1:A:20:GLY:H	1:A:28:GLN:NE2	2.14	0.45
1:B:130:LEU:HG	1:B:150:ALA:HB3	1.98	0.45
1:B:164:ILE:HG23	1:B:164:ILE:O	2.16	0.45
1:B:164:ILE:HD13	1:B:170:LEU:HD22	1.99	0.45
1:C:130:LEU:HD12	1:C:130:LEU:N	2.32	0.45
1:D:185:ALA:HB3	2:D:307:HOH:O	2.16	0.45
1:D:189:SER:HB2	1:D:190:PRO:HD2	1.99	0.45
1:A:21:LYS:N	1:A:21:LYS:HD3	2.32	0.44
1:B:152:MSE:CG	1:B:182:ILE:HG23	2.43	0.44
1:D:18:GLY:HA2	1:D:41:THR:HG22	1.98	0.44
1:A:130:LEU:N	1:A:130:LEU:HD12	2.33	0.44
1:B:3:MSE:HE2	1:B:10:SER:CB	2.47	0.44
1:C:44:VAL:HG21	1:C:88:ALA:HB2	2.00	0.44
1:C:16:LEU:HG	1:C:39:ILE:HB	1.98	0.44
1:D:170:LEU:O	1:D:174:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ILE:HG23	2:D:403:HOH:O	2.17	0.44
1:B:129:VAL:C	1:B:130:LEU:HD12	2.38	0.44
1:C:185:ALA:HB1	2:C:332:HOH:O	2.16	0.44
1:C:17:LEU:HD12	1:C:206:LEU:HD12	2.00	0.44
1:A:130:LEU:HG	1:A:150:ALA:HB3	1.99	0.43
1:B:141:ARG:O	1:B:145:GLU:HG3	2.17	0.43
1:A:3:MSE:HE2	1:A:10:SER:CB	2.48	0.43
1:D:152:MSE:HG2	1:D:182:ILE:HG23	2.00	0.43
1:B:130:LEU:N	1:B:130:LEU:HD12	2.34	0.42
1:C:174:ILE:HG12	1:C:174:ILE:H	1.73	0.42
1:A:241:LEU:HD13	1:C:250:PRO:HG2	2.01	0.42
1:A:102:ILE:HD12	1:A:108:LEU:O	2.19	0.42
1:B:16:LEU:HG	1:B:39:ILE:HB	2.01	0.42
1:C:138:VAL:O	1:C:142:LYS:HG2	2.19	0.42
1:A:16:LEU:HG	1:A:39:ILE:HB	2.01	0.42
1:A:151:ILE:CD1	1:A:181:VAL:HG22	2.46	0.42
1:C:171:SER:O	1:C:174:ILE:HG12	2.20	0.42
1:A:205:LEU:C	1:A:205:LEU:HD23	2.41	0.41
1:B:156:SER:HB3	1:B:165:LEU:HG	2.02	0.41
1:B:241:LEU:CD1	1:D:250:PRO:HB2	2.50	0.41
1:C:130:LEU:HG	1:C:150:ALA:HB3	2.00	0.41
1:D:156:SER:HB2	1:D:157:PRO:CD	2.50	0.41
1:A:107:SER:O	1:A:108:LEU:HB2	2.21	0.41
1:A:190:PRO:HG2	1:B:233:SER:HB2	2.02	0.41
1:D:205:LEU:HD23	1:D:205:LEU:C	2.40	0.41
1:A:245:GLY:HA2	1:A:252:GLU:O	2.20	0.41
1:B:170:LEU:O	1:B:174:ILE:HG12	2.20	0.41
1:C:77:THR:OG1	1:C:80:GLU:HG3	2.19	0.41
1:A:61:LEU:O	1:A:63:LEU:HD12	2.20	0.41
1:C:170:LEU:O	1:C:174:ILE:HG12	2.21	0.41
1:A:129:VAL:C	1:A:130:LEU:HD12	2.41	0.41
1:A:189:SER:HB2	1:A:190:PRO:HD2	2.02	0.41
1:D:49:ILE:HB	1:D:87:LEU:HD21	2.03	0.41
1:B:68:LEU:HD22	1:B:68:LEU:N	2.36	0.41
1:B:70:PRO:HD2	1:B:96:MSE:O	2.21	0.41
1:D:174:ILE:HG12	1:D:174:ILE:H	1.70	0.41
1:D:51:GLU:HG2	1:D:52:ALA:N	2.30	0.41
1:D:48:ASN:HB3	1:D:54:GLN:O	2.21	0.40
1:A:152:MSE:CG	1:A:182:ILE:HG23	2.49	0.40
1:C:19:THR:HB	1:C:28:GLN:NE2	2.37	0.40
1:C:187:ILE:HG23	1:C:192:ASP:HB2	2.04	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	240/264 (91%)	234 (98%)	5 (2%)	1 (0%)	34 21
1	B	249/264 (94%)	239 (96%)	9 (4%)	1 (0%)	34 21
1	C	247/264 (94%)	242 (98%)	4 (2%)	1 (0%)	34 21
1	D	247/264 (94%)	238 (96%)	8 (3%)	1 (0%)	34 21
All	All	983/1056 (93%)	953 (97%)	26 (3%)	4 (0%)	34 21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	49	ILE
1	B	185	ALA
1	C	185	ALA
1	A	185	ALA

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	194/205 (95%)	190 (98%)	4 (2%)	53 42
1	B	200/205 (98%)	197 (98%)	3 (2%)	65 56
1	C	199/205 (97%)	196 (98%)	3 (2%)	65 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	199/205 (97%)	191 (96%)	8 (4%)	31 16
All	All	792/820 (97%)	774 (98%)	18 (2%)	50 37

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

Mol	Chain	Res	Type
1	A	21	LYS
1	A	116	LEU
1	A	182	ILE
1	A	241	LEU
1	B	44	VAL
1	B	174	ILE
1	B	182	ILE
1	C	45	ARG
1	C	116	LEU
1	C	207	ASN
1	D	21	LYS
1	D	45	ARG
1	D	50	PHE
1	D	116	LEU
1	D	164	ILE
1	D	174	ILE
1	D	206	LEU
1	D	207	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	60	GLN
1	A	121	GLN
1	A	243	GLN
1	B	28	GLN
1	B	60	GLN
1	B	121	GLN
1	B	243	GLN
1	C	12	GLN
1	C	28	GLN
1	C	54	GLN
1	C	56	ASN
1	C	60	GLN

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Mol	Chain	Res	Type
1	C	121	GLN
1	C	162	GLN
1	D	28	GLN
1	D	54	GLN
1	D	60	GLN
1	D	207	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	237/264 (89%)	0.16	16 (6%)	17	13	12, 20, 46, 57	0
1	B	244/264 (92%)	0.35	24 (9%)	7	5	12, 19, 47, 56	0
1	C	242/264 (91%)	0.16	14 (5%)	23	18	11, 20, 40, 53	0
1	D	242/264 (91%)	0.21	12 (4%)	28	23	11, 19, 34, 47	0
All	All	965/1056 (91%)	0.22	66 (6%)	17	13	11, 19, 42, 57	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	PHE	13.9
1	D	51	GLU	11.0
1	B	55	PRO	10.8
1	C	2	SER	8.3
1	B	53	SER	7.6
1	A	2	SER	7.5
1	B	54	GLN	6.6
1	D	52	ALA	6.5
1	B	57	PHE	6.2
1	B	251	GLY	6.1
1	D	2	SER	6.0
1	A	50	PHE	5.9
1	B	46	ARG	5.3
1	A	59	GLU	5.3
1	B	252	GLU	4.6
1	B	52	ALA	4.5
1	B	59	GLU	4.4
1	B	56	ASN	4.3
1	C	59	GLU	4.2
1	A	63	LEU	4.2
1	B	2	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	51	GLU	4.0
1	A	60	GLN	4.0
1	A	48	ASN	3.9
1	B	49	ILE	3.9
1	B	48	ASN	3.8
1	C	243	GLN	3.7
1	C	52	ALA	3.7
1	A	252	GLU	3.7
1	A	49	ILE	3.7
1	D	53	SER	3.6
1	A	243	GLN	3.5
1	B	64	SER	3.5
1	A	251	GLY	3.5
1	B	50	PHE	3.5
1	B	243	GLN	3.4
1	C	55	PRO	3.3
1	C	57	PHE	3.2
1	C	46	ARG	3.2
1	A	25	PHE	3.0
1	B	58	LEU	3.0
1	B	249	SER	3.0
1	D	243	GLN	2.9
1	A	58	LEU	2.8
1	D	206	LEU	2.7
1	B	60	GLN	2.7
1	C	53	SER	2.7
1	C	48	ASN	2.6
1	A	46	ARG	2.6
1	B	25	PHE	2.6
1	B	65	LYS	2.5
1	D	249	SER	2.4
1	B	51	GLU	2.4
1	C	249	SER	2.3
1	C	185	ALA	2.3
1	D	182	ILE	2.3
1	B	174	ILE	2.3
1	D	45	ARG	2.3
1	D	46	ARG	2.3
1	B	8	GLY	2.2
1	A	174	ILE	2.2
1	D	174	ILE	2.2
1	A	44	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	25	PHE	2.2
1	A	164	ILE	2.1
1	C	182	ILE	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.