Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:52 pm BST

PDB ID	:	2QKO
Title	:	Crystal structure of transcriptional regulator RHA06399 from Rhodococcus sp. RHA1
Authors	:	Chang, C.; Xu, X.; Zheng, H.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2007-07-11
Resolution	:	2.35 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:

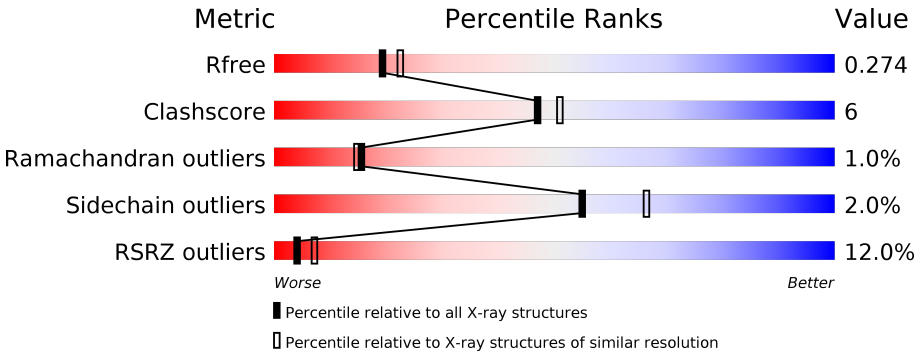
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	215	15% 70% 11% 19%
1	B	215	11% 67% 13% 18%
1	C	215	% 71% 10% 18%
1	D	215	11% 66% 16% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5480 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 Possible transcriptional regulator, TetR family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	Se	0	0	0
			1333	834	243	253	3			
1	B	176	Total	C	N	O	Se	0	0	0
			1350	843	247	257	3			
1	C	176	Total	C	N	O	Se	0	0	0
			1350	843	247	257	3			
1	D	176	Total	C	N	O	Se	0	0	0
			1350	843	247	257	3			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	CLONING ARTIFACT	UNP Q0S912
A	-20	GLY	-	CLONING ARTIFACT	UNP Q0S912
A	-19	SER	-	CLONING ARTIFACT	UNP Q0S912
A	-18	SER	-	CLONING ARTIFACT	UNP Q0S912
A	-17	HIS	-	CLONING ARTIFACT	UNP Q0S912
A	-16	HIS	-	CLONING ARTIFACT	UNP Q0S912
A	-15	HIS	-	CLONING ARTIFACT	UNP Q0S912
A	-14	HIS	-	CLONING ARTIFACT	UNP Q0S912
A	-13	HIS	-	CLONING ARTIFACT	UNP Q0S912
A	-12	HIS	-	CLONING ARTIFACT	UNP Q0S912
A	-11	SER	-	CLONING ARTIFACT	UNP Q0S912
A	-10	SER	-	CLONING ARTIFACT	UNP Q0S912
A	-9	GLY	-	CLONING ARTIFACT	UNP Q0S912
A	-8	ARG	-	CLONING ARTIFACT	UNP Q0S912
A	-7	GLU	-	CLONING ARTIFACT	UNP Q0S912
A	-6	ASN	-	CLONING ARTIFACT	UNP Q0S912
A	-5	LEU	-	CLONING ARTIFACT	UNP Q0S912
A	-4	TYR	-	CLONING ARTIFACT	UNP Q0S912
A	-3	PHE	-	CLONING ARTIFACT	UNP Q0S912
A	-2	GLN	-	CLONING ARTIFACT	UNP Q0S912
A	-1	GLY	-	CLONING ARTIFACT	UNP Q0S912

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	CLONING ARTIFACT	UNP Q0S912
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
A	89	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
A	152	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
A	157	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
B	-21	MSE	-	CLONING ARTIFACT	UNP Q0S912
B	-20	GLY	-	CLONING ARTIFACT	UNP Q0S912
B	-19	SER	-	CLONING ARTIFACT	UNP Q0S912
B	-18	SER	-	CLONING ARTIFACT	UNP Q0S912
B	-17	HIS	-	CLONING ARTIFACT	UNP Q0S912
B	-16	HIS	-	CLONING ARTIFACT	UNP Q0S912
B	-15	HIS	-	CLONING ARTIFACT	UNP Q0S912
B	-14	HIS	-	CLONING ARTIFACT	UNP Q0S912
B	-13	HIS	-	CLONING ARTIFACT	UNP Q0S912
B	-12	HIS	-	CLONING ARTIFACT	UNP Q0S912
B	-11	SER	-	CLONING ARTIFACT	UNP Q0S912
B	-10	SER	-	CLONING ARTIFACT	UNP Q0S912
B	-9	GLY	-	CLONING ARTIFACT	UNP Q0S912
B	-8	ARG	-	CLONING ARTIFACT	UNP Q0S912
B	-7	GLU	-	CLONING ARTIFACT	UNP Q0S912
B	-6	ASN	-	CLONING ARTIFACT	UNP Q0S912
B	-5	LEU	-	CLONING ARTIFACT	UNP Q0S912
B	-4	TYR	-	CLONING ARTIFACT	UNP Q0S912
B	-3	PHE	-	CLONING ARTIFACT	UNP Q0S912
B	-2	GLN	-	CLONING ARTIFACT	UNP Q0S912
B	-1	GLY	-	CLONING ARTIFACT	UNP Q0S912
B	0	HIS	-	CLONING ARTIFACT	UNP Q0S912
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
B	89	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
B	152	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
B	157	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
C	-21	MSE	-	CLONING ARTIFACT	UNP Q0S912
C	-20	GLY	-	CLONING ARTIFACT	UNP Q0S912
C	-19	SER	-	CLONING ARTIFACT	UNP Q0S912
C	-18	SER	-	CLONING ARTIFACT	UNP Q0S912
C	-17	HIS	-	CLONING ARTIFACT	UNP Q0S912
C	-16	HIS	-	CLONING ARTIFACT	UNP Q0S912
C	-15	HIS	-	CLONING ARTIFACT	UNP Q0S912
C	-14	HIS	-	CLONING ARTIFACT	UNP Q0S912
C	-13	HIS	-	CLONING ARTIFACT	UNP Q0S912
C	-12	HIS	-	CLONING ARTIFACT	UNP Q0S912
C	-11	SER	-	CLONING ARTIFACT	UNP Q0S912

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	SER	-	CLONING ARTIFACT	UNP Q0S912
C	-9	GLY	-	CLONING ARTIFACT	UNP Q0S912
C	-8	ARG	-	CLONING ARTIFACT	UNP Q0S912
C	-7	GLU	-	CLONING ARTIFACT	UNP Q0S912
C	-6	ASN	-	CLONING ARTIFACT	UNP Q0S912
C	-5	LEU	-	CLONING ARTIFACT	UNP Q0S912
C	-4	TYR	-	CLONING ARTIFACT	UNP Q0S912
C	-3	PHE	-	CLONING ARTIFACT	UNP Q0S912
C	-2	GLN	-	CLONING ARTIFACT	UNP Q0S912
C	-1	GLY	-	CLONING ARTIFACT	UNP Q0S912
C	0	HIS	-	CLONING ARTIFACT	UNP Q0S912
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
C	89	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
C	152	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
C	157	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
D	-21	MSE	-	CLONING ARTIFACT	UNP Q0S912
D	-20	GLY	-	CLONING ARTIFACT	UNP Q0S912
D	-19	SER	-	CLONING ARTIFACT	UNP Q0S912
D	-18	SER	-	CLONING ARTIFACT	UNP Q0S912
D	-17	HIS	-	CLONING ARTIFACT	UNP Q0S912
D	-16	HIS	-	CLONING ARTIFACT	UNP Q0S912
D	-15	HIS	-	CLONING ARTIFACT	UNP Q0S912
D	-14	HIS	-	CLONING ARTIFACT	UNP Q0S912
D	-13	HIS	-	CLONING ARTIFACT	UNP Q0S912
D	-12	HIS	-	CLONING ARTIFACT	UNP Q0S912
D	-11	SER	-	CLONING ARTIFACT	UNP Q0S912
D	-10	SER	-	CLONING ARTIFACT	UNP Q0S912
D	-9	GLY	-	CLONING ARTIFACT	UNP Q0S912
D	-8	ARG	-	CLONING ARTIFACT	UNP Q0S912
D	-7	GLU	-	CLONING ARTIFACT	UNP Q0S912
D	-6	ASN	-	CLONING ARTIFACT	UNP Q0S912
D	-5	LEU	-	CLONING ARTIFACT	UNP Q0S912
D	-4	TYR	-	CLONING ARTIFACT	UNP Q0S912
D	-3	PHE	-	CLONING ARTIFACT	UNP Q0S912
D	-2	GLN	-	CLONING ARTIFACT	UNP Q0S912
D	-1	GLY	-	CLONING ARTIFACT	UNP Q0S912
D	0	HIS	-	CLONING ARTIFACT	UNP Q0S912
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
D	89	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
D	152	MSE	MET	MODIFIED RESIDUE	UNP Q0S912
D	157	MSE	MET	MODIFIED RESIDUE	UNP Q0S912

- Molecule 2 is water.

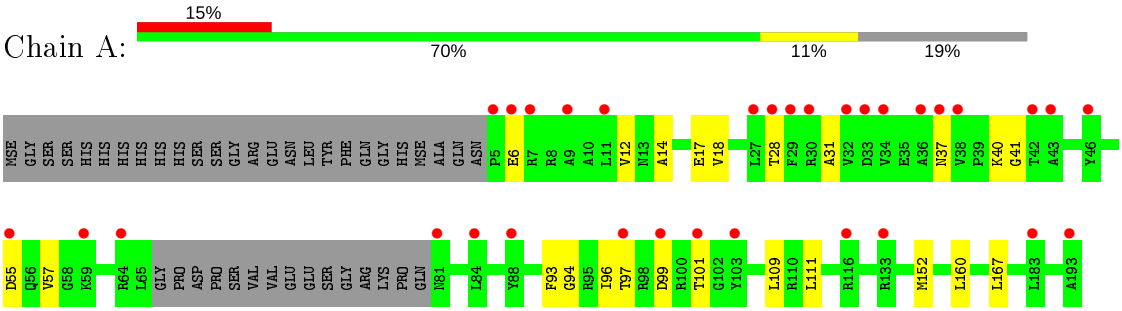
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0
2	B	22	Total O 22 22	0	0
2	C	22	Total O 22 22	0	0
2	D	27	Total O 27 27	0	0

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.

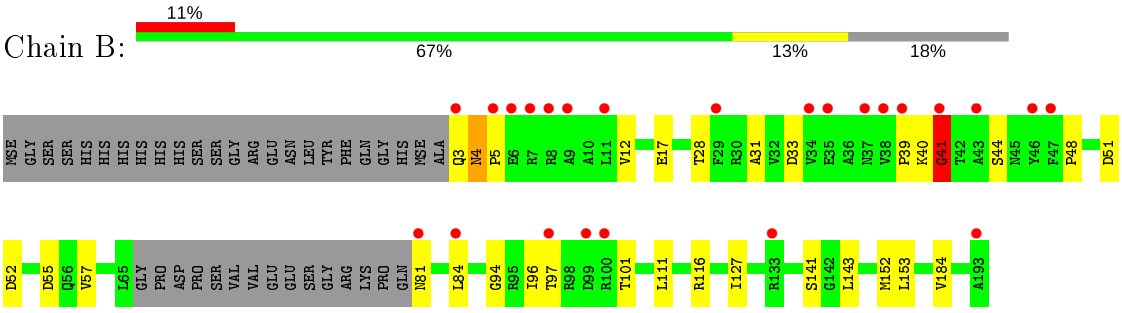
- Molecule 1: Possible transcriptional regulator, TetR family protein

Chain A:



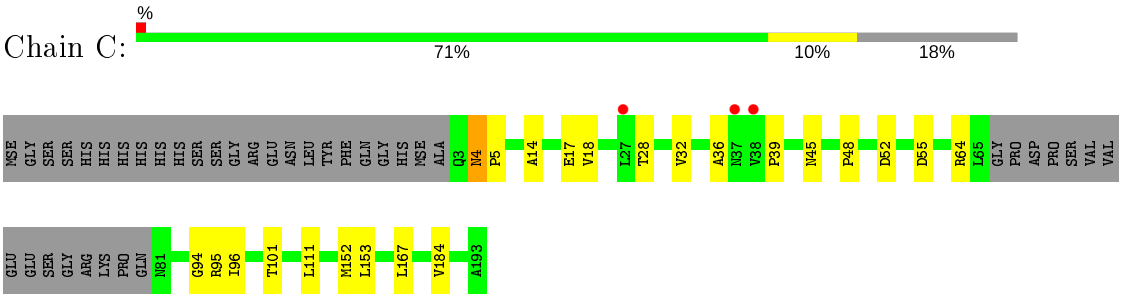
- Molecule 1: Possible transcriptional regulator, TetR family protein

Chain B:



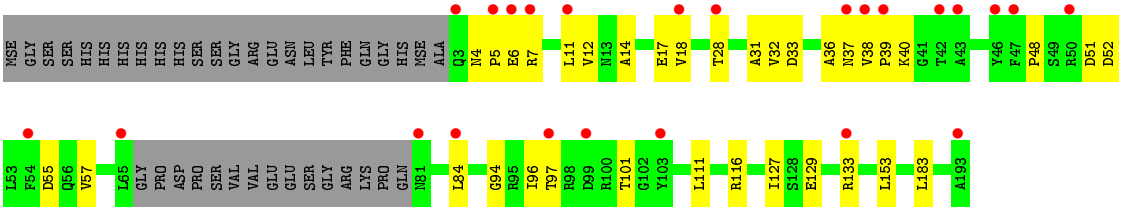
- Molecule 1: Possible transcriptional regulator, TetR family protein

Chain C:



- Molecule 1: Possible transcriptional regulator, TetR family protein

Chain D:


MSE GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU GLU ASN LEU TYR PHE GLN GLY HIS MSE ALA Q3 N4 P5 E6 R7 L11 V12 N13 A14 E17 V18 T28 A31 V32 D33 A36 N37 V38 P39 K40 G41 T42 A43 Y46 F47 P48 S49 R50 D51 D52
L53 F54 D55 Q56 V57 L65 GLY PRO ASP PRO SER VAL VAL GLU GLU SER GLY ARG LYS PRO GLN N81 L84 G94 R95 I96 T97 R98 D99 R100 T101 G102 Y103 L111 R116 I127 S128 E129 R133 L153 L183 A193

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	62.31Å 62.31Å 164.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.43 – 2.35 38.43 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.43-2.35) 99.7 (38.43-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.73 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.273 0.232 , 0.274	Depositor DCC
R_{free} test set	1502 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.488 for -h,-k,l 0.488 for h,-h-k,-l 0.487 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5480	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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	0.70	4/1347 (0.3%)	0.63	0/1822
1	B	0.69	4/1364 (0.3%)	0.67	1/1846 (0.1%)
1	C	0.51	0/1364	0.63	0/1846
1	D	0.55	2/1364 (0.1%)	0.62	0/1846
All	All	0.62	10/5439 (0.2%)	0.64	1/7360 (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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	GLU	CD-OE2	15.30	1.42	1.25
1	B	81	ASN	CG-ND2	9.32	1.56	1.32
1	B	41	GLY	C-N	8.32	1.53	1.34
1	B	40	LYS	C-O	8.04	1.38	1.23
1	D	6	GLU	CD-OE2	6.82	1.33	1.25
1	B	81	ASN	CG-OD1	6.29	1.37	1.24
1	D	6	GLU	CD-OE1	5.55	1.31	1.25
1	A	6	GLU	CD-OE1	5.38	1.31	1.25
1	A	40	LYS	C-O	5.12	1.33	1.23
1	A	40	LYS	C-N	5.02	1.42	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	41	GLY	CA-C-N	-6.68	102.50	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	41	GLY	Mainchain

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	1333	0	1332	20	0
1	B	1350	0	1345	25	0
1	C	1350	0	1345	14	0
1	D	1350	0	1345	21	0
2	A	26	0	0	0	0
2	B	22	0	0	1	0
2	C	22	0	0	0	0
2	D	27	0	0	0	0
All	All	5480	0	5367	66	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 6.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MSE:HE3	1:B:152:MSE:CE	1.37	1.50
1:A:152:MSE:CE	1:B:152:MSE:HE1	1.50	1.41
1:A:152:MSE:HE3	1:B:152:MSE:HE3	1.17	1.08
1:A:152:MSE:HE1	1:B:152:MSE:HE1	1.47	0.95
1:C:28:THR:O	1:C:32:VAL:HG23	1.71	0.90
1:C:14:ALA:O	1:C:18:VAL:HG23	1.87	0.73
1:A:152:MSE:HE2	1:B:152:MSE:HE1	1.66	0.71
1:D:36:ALA:C	1:D:38:VAL:H	1.98	0.66
1:A:17:GLU:OE2	1:A:101:THR:HG21	1.97	0.65
1:B:3:GLN:N	2:B:207:HOH:O	2.29	0.64
1:C:111:LEU:HD12	1:D:111:LEU:HD12	1.80	0.63
1:B:96:ILE:HG23	1:B:97:THR:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD12	1:B:111:LEU:HD12	1.81	0.61
1:B:141:SER:OG	1:B:143:LEU:HD12	2.01	0.60
1:B:4:ASN:HB3	1:B:5:PRO:CD	2.34	0.57
1:B:4:ASN:HB3	1:B:5:PRO:HD3	1.87	0.56
1:C:4:ASN:H	1:C:5:PRO:HD2	1.69	0.56
1:A:152:MSE:HE3	1:B:152:MSE:HE2	1.66	0.56
1:D:33:ASP:O	1:D:39:PRO:HA	2.05	0.56
1:B:94:GLY:C	1:B:96:ILE:H	2.09	0.56
1:D:96:ILE:HG23	1:D:97:THR:N	2.22	0.54
1:B:17:GLU:OE2	1:B:101:THR:HG21	2.08	0.54
1:A:111:LEU:HD12	1:B:111:LEU:CD1	2.39	0.53
1:D:17:GLU:OE2	1:D:101:THR:HG21	2.09	0.52
1:B:28:THR:HG23	1:B:31:ALA:H	1.75	0.51
1:A:152:MSE:CE	1:B:152:MSE:HE3	2.04	0.51
1:A:28:THR:HG23	1:A:31:ALA:H	1.76	0.51
1:C:17:GLU:OE2	1:C:64:ARG:NH2	2.44	0.51
1:D:94:GLY:C	1:D:96:ILE:H	2.15	0.50
1:C:48:PRO:HD2	1:C:52:ASP:OD2	2.12	0.49
1:C:111:LEU:CD1	1:D:111:LEU:HD12	2.43	0.48
1:A:14:ALA:O	1:A:18:VAL:HG23	2.14	0.48
1:D:12:VAL:HG13	1:D:57:VAL:HG22	1.96	0.48
1:B:96:ILE:HG23	1:B:97:THR:H	1.79	0.48
1:D:36:ALA:C	1:D:38:VAL:N	2.66	0.47
1:A:96:ILE:HG23	1:A:97:THR:N	2.30	0.47
1:D:153:LEU:CD2	1:D:183:LEU:HG	2.44	0.47
1:B:12:VAL:HG13	1:B:57:VAL:HG22	1.96	0.46
1:C:4:ASN:H	1:C:5:PRO:CD	2.28	0.46
1:B:48:PRO:HD2	1:B:52:ASP:OD2	2.16	0.46
1:B:96:ILE:CG2	1:B:97:THR:N	2.79	0.46
1:D:129:GLU:O	1:D:133:ARG:HG3	2.15	0.45
1:C:94:GLY:C	1:C:96:ILE:H	2.20	0.45
1:C:111:LEU:HD12	1:D:111:LEU:CD1	2.46	0.45
1:D:32:VAL:O	1:D:36:ALA:N	2.49	0.45
1:B:51:ASP:HA	1:B:116:ARG:NH1	2.33	0.44
1:A:93:PHE:O	1:A:96:ILE:CG2	2.67	0.43
1:D:28:THR:HG23	1:D:31:ALA:H	1.83	0.43
1:D:7:ARG:O	1:D:11:LEU:HG	2.18	0.43
1:B:33:ASP:O	1:B:39:PRO:HA	2.19	0.43
1:A:57:VAL:HG12	1:A:109:LEU:HD11	2.01	0.43
1:C:153:LEU:HD21	1:C:184:VAL:HA	2.01	0.43
1:A:12:VAL:HG13	1:A:57:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:O	1:A:96:ILE:HG22	2.19	0.43
1:C:17:GLU:OE2	1:C:101:THR:HG21	2.19	0.43
1:A:93:PHE:CE1	1:A:160:LEU:HG	2.54	0.42
1:D:4:ASN:N	1:D:5:PRO:CD	2.82	0.42
1:C:36:ALA:O	1:C:39:PRO:HG3	2.20	0.42
1:D:51:ASP:HA	1:D:116:ARG:NH1	2.35	0.42
1:D:14:ALA:O	1:D:18:VAL:HG23	2.19	0.42
1:D:153:LEU:HD23	1:D:153:LEU:HA	1.91	0.41
1:A:94:GLY:C	1:A:96:ILE:H	2.23	0.41
1:D:48:PRO:HD2	1:D:52:ASP:OD2	2.21	0.41
1:A:167:LEU:CD1	1:B:127:ILE:HD12	2.51	0.41
1:B:153:LEU:HD21	1:B:184:VAL:HA	2.04	0.40
1:C:167:LEU:CD1	1:D:127:ILE:HD12	2.52	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	170/215 (79%)	165 (97%)	4 (2%)	1 (1%)	25	27
1	B	172/215 (80%)	165 (96%)	5 (3%)	2 (1%)	13	11
1	C	172/215 (80%)	162 (94%)	8 (5%)	2 (1%)	13	11
1	D	172/215 (80%)	162 (94%)	8 (5%)	2 (1%)	13	11
All	All	686/860 (80%)	654 (95%)	25 (4%)	7 (1%)	15	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	37	ASN
1	D	40	LYS

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Mol	Chain	Res	Type
1	C	4	ASN
1	B	4	ASN
1	B	41	GLY
1	C	95	ARG
1	A	41	GLY

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	137/174 (79%)	134 (98%)	3 (2%)	52	63
1	B	139/174 (80%)	136 (98%)	3 (2%)	52	63
1	C	139/174 (80%)	136 (98%)	3 (2%)	52	63
1	D	139/174 (80%)	137 (99%)	2 (1%)	67	78
All	All	554/696 (80%)	543 (98%)	11 (2%)	55	66

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	55	ASP
1	A	99	ASP
1	B	44	SER
1	B	55	ASP
1	B	84	LEU
1	C	45	ASN
1	C	55	ASP
1	C	152	MSE
1	D	55	ASP
1	D	84	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	171/215 (79%)	1.07	32 (18%) 1 2	36, 54, 76, 83	0
1	B	173/215 (80%)	0.98	24 (13%) 2 4	37, 53, 77, 82	0
1	C	173/215 (80%)	0.03	3 (1%) 70 78	34, 59, 88, 103	0
1	D	173/215 (80%)	1.03	24 (13%) 2 4	36, 53, 77, 84	0
All	All	690/860 (80%)	0.77	83 (12%) 4 7	34, 55, 81, 103	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ASN	12.2
1	D	37	ASN	11.4
1	B	37	ASN	9.3
1	D	3	GLN	9.3
1	A	38	VAL	9.1
1	B	193	ALA	9.0
1	B	3	GLN	8.2
1	D	38	VAL	7.2
1	A	5	PRO	7.1
1	D	5	PRO	7.0
1	B	38	VAL	6.5
1	C	37	ASN	6.1
1	B	43	ALA	5.0
1	B	7	ARG	5.0
1	B	5	PRO	4.9
1	A	193	ALA	4.9
1	D	193	ALA	4.8
1	C	38	VAL	4.8
1	A	29	PHE	4.5
1	B	6	GLU	4.4
1	D	43	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	46	TYR	4.1
1	D	81	ASN	4.0
1	A	11	LEU	3.9
1	A	6	GLU	3.8
1	B	9	ALA	3.4
1	D	42	THR	3.3
1	A	32	VAL	3.2
1	A	7	ARG	3.2
1	A	84	LEU	3.1
1	A	36	ALA	3.1
1	A	9	ALA	3.1
1	B	84	LEU	3.0
1	A	27	LEU	3.0
1	D	99	ASP	3.0
1	A	59	LYS	3.0
1	D	7	ARG	2.9
1	A	43	ALA	2.9
1	A	133	ARG	2.8
1	D	6	GLU	2.8
1	D	46	TYR	2.8
1	D	18	VAL	2.7
1	A	97	THR	2.7
1	A	34	VAL	2.7
1	D	133	ARG	2.7
1	B	46	TYR	2.7
1	D	54	PHE	2.6
1	D	65	LEU	2.6
1	D	103	TYR	2.5
1	A	28	THR	2.5
1	B	39	PRO	2.5
1	B	29	PHE	2.5
1	A	30	ARG	2.5
1	B	100	ARG	2.5
1	D	11	LEU	2.5
1	A	99	ASP	2.5
1	B	133	ARG	2.4
1	B	11	LEU	2.4
1	D	47	PHE	2.4
1	A	81	ASN	2.3
1	A	42	THR	2.3
1	D	50	ARG	2.3
1	A	55	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	28	THR	2.3
1	B	47	PHE	2.3
1	A	101	THR	2.2
1	B	97	THR	2.2
1	A	33	ASP	2.2
1	A	103	TYR	2.2
1	C	27	LEU	2.2
1	A	88	TYR	2.2
1	B	35	GLU	2.2
1	B	99	ASP	2.2
1	D	39	PRO	2.1
1	A	64	ARG	2.1
1	B	8	ARG	2.1
1	B	34	VAL	2.1
1	A	116	ARG	2.0
1	B	81	ASN	2.0
1	D	84	LEU	2.0
1	D	97	THR	2.0
1	A	183	LEU	2.0
1	B	41	GLY	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 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.