Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 11:03 AM BST

PDB ID	:	2I15
Title	:	Crystal structure of MPN423 from Mycoplasma pneumoniae
Authors	:	Shin, D.H.; Yokota, H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	2006-08-12
Resolution	:	2.40 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:

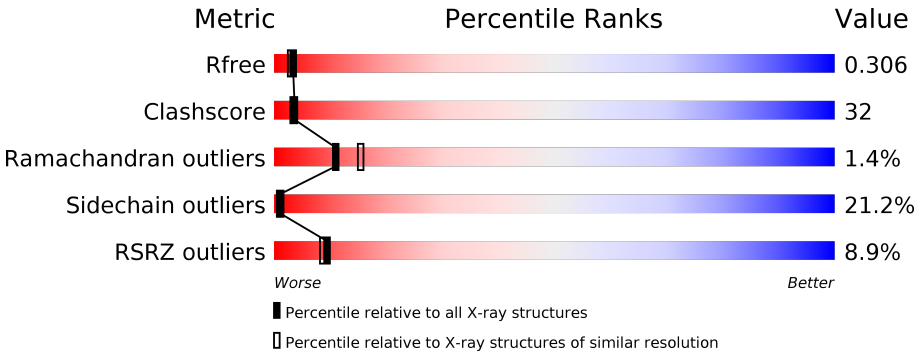
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	135	10% 37% 39% 14% • 10%
1	B	135	9% 39% 39% 13% 10%
1	C	135	4% 36% 39% 10% • 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3028 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hypothetical protein MG296 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			1002	647	160	190	5			
1	B	122	Total	C	N	O	S	0	0	0
			1002	647	160	190	5			
1	C	115	Total	C	N	O	S	0	0	0
			950	614	152	179	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	cloning artifact	UNP P75364
A	-4	GLY	-	cloning artifact	UNP P75364
A	-3	GLY	-	cloning artifact	UNP P75364
A	-2	GLY	-	cloning artifact	UNP P75364
A	-1	GLY	-	cloning artifact	UNP P75364
A	0	GLY	-	cloning artifact	UNP P75364
B	195	GLY	-	cloning artifact	UNP P75364
B	196	GLY	-	cloning artifact	UNP P75364
B	197	GLY	-	cloning artifact	UNP P75364
B	198	GLY	-	cloning artifact	UNP P75364
B	199	GLY	-	cloning artifact	UNP P75364
B	200	GLY	-	cloning artifact	UNP P75364
C	395	GLY	-	cloning artifact	UNP P75364
C	396	GLY	-	cloning artifact	UNP P75364
C	397	GLY	-	cloning artifact	UNP P75364
C	398	GLY	-	cloning artifact	UNP P75364
C	399	GLY	-	cloning artifact	UNP P75364
C	400	GLY	-	cloning artifact	UNP P75364

- Molecule 2 is water.

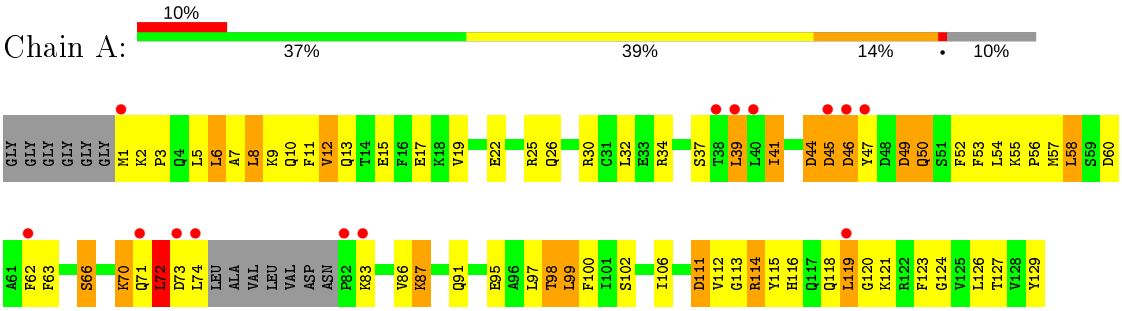
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	21	Total O 21 21	0	0
2	C	26	Total O 26 26	0	0

3 Residue-property plots (i)

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

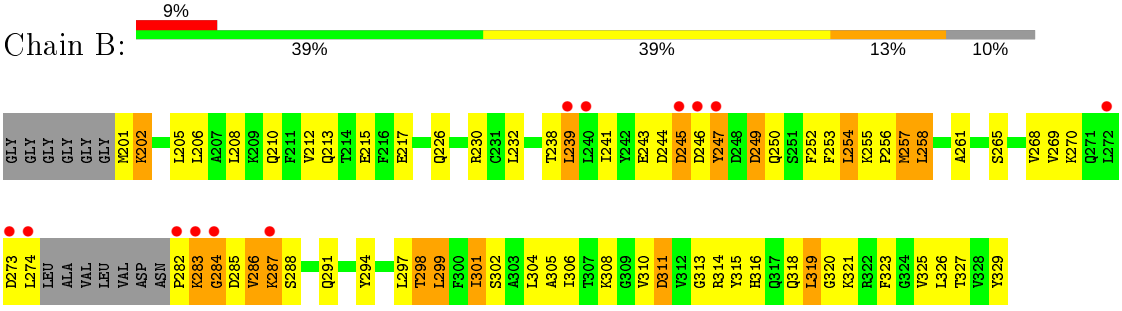
• Molecule 1: Hypothetical protein MG296 homolog

Chain A:



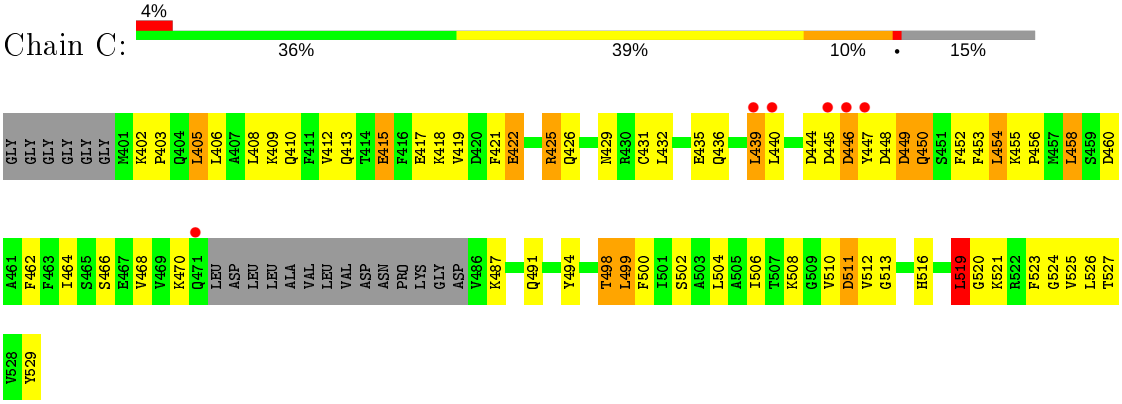
• Molecule 1: Hypothetical protein MG296 homolog

Chain B:



• Molecule 1: Hypothetical protein MG296 homolog

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.13Å 87.58Å 49.93Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40 48.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	78.7 (19.98-2.40) 92.2 (48.77-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.291 0.247 , 0.306	Depositor DCC
R_{free} test set	1625 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3028	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% 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	0.47	0/1021	0.84	3/1370 (0.2%)
1	B	0.50	0/1021	0.84	4/1370 (0.3%)
1	C	0.45	0/968	0.78	3/1299 (0.2%)
All	All	0.47	0/3010	0.82	10/4039 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284	GLY	N-CA-C	-10.04	87.99	113.10
1	A	45	ASP	N-CA-C	-8.98	86.75	111.00
1	A	72	LEU	N-CA-C	-8.75	87.38	111.00
1	C	445	ASP	N-CA-C	-7.85	89.80	111.00
1	B	245	ASP	N-CA-C	-7.85	89.81	111.00
1	B	299	LEU	CA-CB-CG	6.71	130.74	115.30
1	A	46	ASP	N-CA-C	-6.24	94.15	111.00
1	C	446	ASP	N-CA-C	-5.61	95.85	111.00
1	B	247	TYR	N-CA-C	-5.25	96.83	111.00
1	C	519	LEU	CA-CB-CG	5.03	126.87	115.30

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	1002	0	990	85	0
1	B	1002	0	987	45	0
1	C	950	0	933	77	0
2	A	27	0	0	2	0
2	B	21	0	0	2	0
2	C	26	0	0	1	0
All	All	3028	0	2910	185	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 32.

All (185) 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:450:GLN:HE22	1:C:452:PHE:HB3	1.04	1.11
1:A:6:LEU:HG	1:A:7:ALA:N	1.73	1.02
1:C:455:LYS:HB3	1:C:456:PRO:HD3	1.40	1.01
1:A:91:GLN:HE22	1:A:126:LEU:H	1.11	0.96
1:A:44:ASP:HB3	1:A:46:ASP:HB2	1.45	0.94
1:B:283:LYS:HD3	1:B:284:GLY:O	1.70	0.90
1:C:450:GLN:NE2	1:C:452:PHE:HB3	1.86	0.88
1:B:255:LYS:HE3	1:B:256:PRO:HD3	1.56	0.85
1:A:46:ASP:O	1:A:47:TYR:HB2	1.77	0.83
1:A:34:ARG:HH22	1:C:436:GLN:HE22	1.24	0.82
1:C:449:ASP:OD2	1:C:454:LEU:HD23	1.80	0.81
1:C:491:GLN:HE22	1:C:526:LEU:H	1.23	0.81
1:A:58:LEU:HD11	1:A:100:PHE:CZ	2.17	0.79
1:C:447:TYR:OH	1:C:458:LEU:HD21	1.83	0.78
1:B:291:GLN:HE22	1:B:326:LEU:H	1.31	0.78
1:A:54:LEU:HD12	1:C:421:PHE:HE1	1.49	0.77
1:B:286:VAL:HG13	1:B:287:LYS:H	1.47	0.77
1:A:52:PHE:O	1:A:56:PRO:CD	2.35	0.74
1:A:13:GLN:O	1:A:17:GLU:HG3	1.90	0.72
1:A:55:LYS:HB3	1:A:56:PRO:HD3	1.70	0.72
1:C:470:LYS:O	1:C:470:LYS:HG3	1.90	0.72
1:A:54:LEU:HD12	1:C:421:PHE:CE1	2.26	0.70
1:C:455:LYS:CB	1:C:456:PRO:HD3	2.20	0.70
1:A:73:ASP:O	1:A:74:LEU:HB2	1.92	0.70
1:A:98:THR:HG21	1:C:448:ASP:O	1.92	0.69
1:C:440:LEU:HG	1:C:440:LEU:O	1.92	0.69
1:B:320:GLY:O	1:B:323:PHE:O	2.10	0.69
1:A:91:GLN:O	1:A:95:GLU:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLN:O	1:B:217:GLU:HG3	1.93	0.69
1:B:244:ASP:O	1:B:246:ASP:N	2.26	0.68
1:B:246:ASP:O	1:B:247:TYR:HB2	1.93	0.68
1:A:6:LEU:CG	1:A:7:ALA:N	2.56	0.67
1:A:120:GLY:O	1:A:123:PHE:O	2.13	0.67
1:B:265:SER:O	1:B:269:VAL:HG22	1.95	0.67
1:A:66:SER:HB2	1:C:409:LYS:HD3	1.75	0.67
1:C:450:GLN:HE22	1:C:452:PHE:CB	1.96	0.66
1:A:34:ARG:HH22	1:C:436:GLN:NE2	1.93	0.66
1:A:41:ILE:HD13	1:A:41:ILE:O	1.97	0.65
1:C:444:ASP:O	1:C:446:ASP:N	2.30	0.65
1:C:455:LYS:HZ2	1:C:456:PRO:HG3	1.62	0.64
1:B:252:PHE:O	1:B:256:PRO:CD	2.46	0.64
1:A:44:ASP:O	1:A:46:ASP:N	2.32	0.63
1:C:462:PHE:HZ	1:C:500:PHE:CZ	2.15	0.63
1:C:520:GLY:O	1:C:523:PHE:O	2.16	0.62
1:C:502:SER:O	1:C:506:ILE:HG12	2.00	0.62
1:A:114:ARG:O	1:A:118:GLN:HG3	2.01	0.61
1:C:455:LYS:NZ	1:C:456:PRO:HG3	2.16	0.61
1:B:241:ILE:HG21	1:B:261:ALA:CB	2.31	0.60
1:B:226:GLN:O	1:B:230:ARG:HG3	2.02	0.60
1:A:49:ASP:OD2	1:A:54:LEU:HB2	2.01	0.60
1:B:286:VAL:HG13	1:B:287:LYS:N	2.16	0.60
1:A:53:PHE:O	1:A:56:PRO:HD2	2.01	0.60
1:A:58:LEU:HD11	1:A:100:PHE:HZ	1.66	0.60
1:B:265:SER:HA	1:B:268:VAL:HG22	1.84	0.60
1:B:314:ARG:O	1:B:318:GLN:HG3	2.01	0.60
1:B:241:ILE:HG21	1:B:261:ALA:HB1	1.84	0.59
1:B:302:SER:O	1:B:306:ILE:HG13	2.03	0.59
1:C:516:HIS:O	1:C:527:THR:HG21	2.02	0.59
1:B:250:GLN:HG3	1:B:253:PHE:HB3	1.83	0.59
1:A:47:TYR:HB3	1:C:425:ARG:HG2	1.83	0.59
1:A:116:HIS:O	1:A:127:THR:HG21	2.02	0.59
1:A:74:LEU:C	1:A:74:LEU:HD23	2.22	0.59
1:A:114:ARG:HB2	1:A:114:ARG:HH11	1.68	0.58
1:A:6:LEU:HG	1:A:7:ALA:H	1.63	0.58
1:A:1:MET:CG	1:A:2:LYS:H	2.17	0.58
1:C:452:PHE:O	1:C:456:PRO:CD	2.51	0.58
1:A:53:PHE:C	1:A:56:PRO:HD2	2.24	0.58
1:A:102:SER:O	1:A:106:ILE:HG12	2.04	0.57
1:A:70:LYS:HB3	1:C:405:LEU:HD12	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD13	1:C:402:LYS:HG2	1.85	0.57
1:A:1:MET:CG	1:A:2:LYS:N	2.67	0.57
1:B:316:HIS:O	1:B:327:THR:HG21	2.04	0.57
1:C:513:GLY:HA2	1:C:529:TYR:CB	2.34	0.57
1:A:44:ASP:HB3	1:A:46:ASP:CB	2.29	0.56
1:C:422:GLU:O	1:C:426:GLN:HG3	2.04	0.56
1:A:74:LEU:C	1:A:74:LEU:CD2	2.73	0.56
1:A:52:PHE:O	1:A:56:PRO:HG2	2.07	0.55
1:A:46:ASP:O	1:A:47:TYR:CB	2.50	0.55
1:A:58:LEU:HD11	1:A:100:PHE:CE1	2.40	0.55
1:A:3:PRO:O	1:A:6:LEU:HD23	2.07	0.55
1:A:113:GLY:HA2	1:A:129:TYR:CG	2.41	0.55
1:B:297:LEU:O	1:B:301:ILE:HD13	2.06	0.55
1:A:11:PHE:O	1:A:15:GLU:HB2	2.07	0.55
1:C:498:THR:HG22	1:C:499:LEU:N	2.20	0.54
1:A:22:GLU:HB2	2:A:151:HOH:O	2.07	0.54
1:A:98:THR:HG22	1:A:99:LEU:N	2.23	0.54
1:B:308:LYS:HD3	1:B:310:VAL:HG21	1.89	0.54
1:A:1:MET:HG3	1:A:2:LYS:H	1.72	0.54
1:A:47:TYR:C	1:C:425:ARG:HH11	2.11	0.54
1:A:52:PHE:O	1:A:56:PRO:CG	2.56	0.54
1:A:115:TYR:OH	1:C:415:GLU:HG2	2.08	0.54
1:A:54:LEU:C	1:A:54:LEU:HD13	2.29	0.53
1:B:254:LEU:O	1:B:258:LEU:HB2	2.09	0.53
1:C:446:ASP:O	1:C:447:TYR:HB2	2.09	0.53
1:B:305:ALA:HB2	1:B:315:TYR:CD2	2.44	0.53
1:A:44:ASP:CB	1:A:46:ASP:HB2	2.31	0.52
1:B:252:PHE:O	1:B:256:PRO:HD3	2.09	0.52
1:A:87:LYS:HG3	1:A:124:GLY:O	2.09	0.52
1:C:487:LYS:NZ	1:C:524:GLY:HA3	2.25	0.52
1:C:464:ILE:O	1:C:468:VAL:HG13	2.10	0.51
1:B:294:TYR:CG	1:B:325:VAL:HG11	2.45	0.51
1:A:47:TYR:HB3	1:C:425:ARG:CG	2.41	0.51
1:A:22:GLU:O	1:A:26:GLN:HG3	2.10	0.50
1:B:319:LEU:HD13	1:B:319:LEU:O	2.10	0.50
1:C:458:LEU:HD11	1:C:500:PHE:CE1	2.46	0.50
1:C:526:LEU:C	1:C:526:LEU:HD23	2.32	0.50
1:A:10:GLN:NE2	2:A:147:HOH:O	2.43	0.50
1:A:49:ASP:OD2	1:A:54:LEU:HD23	2.11	0.50
1:B:294:TYR:CZ	1:B:327:THR:HG22	2.46	0.50
1:C:452:PHE:O	1:C:456:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLN:OE1	1:A:52:PHE:HB3	2.12	0.49
1:C:513:GLY:HA2	1:C:529:TYR:HB3	1.93	0.49
1:C:504:LEU:O	1:C:508:LYS:HG2	2.13	0.49
1:A:66:SER:OG	1:C:405:LEU:HD13	2.11	0.49
1:A:47:TYR:C	1:C:425:ARG:NH1	2.66	0.49
1:B:244:ASP:O	1:B:245:ASP:C	2.51	0.49
1:C:462:PHE:CZ	1:C:500:PHE:CZ	3.00	0.48
1:A:53:PHE:CZ	1:A:57:MET:HG3	2.48	0.48
1:B:270:LYS:O	1:B:270:LYS:CG	2.61	0.48
1:C:453:PHE:O	1:C:456:PRO:HD2	2.13	0.48
1:A:71:GLN:O	1:A:83:LYS:O	2.31	0.48
1:C:440:LEU:O	1:C:440:LEU:CG	2.61	0.47
1:C:455:LYS:HB3	1:C:456:PRO:CD	2.28	0.47
1:C:510:VAL:CG1	1:C:511:ASP:N	2.77	0.47
1:B:249:ASP:OD2	1:B:254:LEU:HD23	2.14	0.47
1:C:413:GLN:O	1:C:417:GLU:HG3	2.15	0.47
1:C:494:TYR:CG	1:C:525:VAL:HG11	2.50	0.47
1:A:9:LYS:O	1:A:13:GLN:HB2	2.15	0.47
1:B:253:PHE:C	1:B:256:PRO:HD2	2.36	0.47
1:A:63:PHE:CE2	1:C:409:LYS:NZ	2.82	0.46
1:A:47:TYR:OH	1:A:58:LEU:HD21	2.14	0.46
1:A:47:TYR:HB2	1:C:429:ASN:OD1	2.15	0.46
1:B:298:THR:HG22	1:B:299:LEU:N	2.31	0.46
1:B:305:ALA:HB2	1:B:315:TYR:CG	2.50	0.46
1:B:311:ASP:HB3	2:B:7:HOH:O	2.15	0.46
1:C:510:VAL:HG12	1:C:511:ASP:N	2.30	0.46
1:C:513:GLY:HA2	1:C:529:TYR:CG	2.51	0.46
1:B:304:LEU:O	1:B:308:LYS:HG2	2.17	0.45
1:B:313:GLY:HA2	1:B:329:TYR:CB	2.46	0.45
1:A:66:SER:CB	1:C:409:LYS:HD3	2.44	0.45
1:A:55:LYS:HB3	1:A:55:LYS:NZ	2.32	0.45
1:C:455:LYS:CB	1:C:456:PRO:CD	2.92	0.45
1:A:72:LEU:HD22	1:C:402:LYS:HG3	1.99	0.45
1:A:98:THR:CG2	1:A:99:LEU:N	2.80	0.45
1:B:201:MET:O	1:B:202:LYS:C	2.55	0.45
1:A:86:VAL:HA	1:C:402:LYS:HE2	2.00	0.44
1:C:462:PHE:HZ	1:C:500:PHE:CE2	2.35	0.44
1:A:116:HIS:O	1:A:119:LEU:HB3	2.17	0.44
1:C:491:GLN:NE2	1:C:526:LEU:H	2.04	0.44
1:C:425:ARG:HD2	2:C:43:HOH:O	2.17	0.44
1:A:8:LEU:O	1:A:12:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PHE:CZ	1:B:257:MET:HG2	2.53	0.43
1:C:410:GLN:HA	1:C:410:GLN:OE1	2.18	0.43
1:C:449:ASP:OD2	1:C:453:PHE:HD1	2.02	0.43
1:A:52:PHE:O	1:A:56:PRO:HD3	2.17	0.43
1:B:297:LEU:HB3	1:B:301:ILE:HD13	2.00	0.43
1:C:402:LYS:HA	1:C:403:PRO:HD3	1.86	0.43
1:C:511:ASP:C	1:C:512:VAL:O	2.53	0.43
1:C:454:LEU:HA	1:C:454:LEU:HD22	1.82	0.43
1:A:1:MET:HG2	1:A:2:LYS:N	2.32	0.42
1:B:246:ASP:HB3	1:B:247:TYR:HD1	1.85	0.42
1:C:450:GLN:NE2	1:C:452:PHE:CB	2.70	0.42
1:A:111:ASP:C	1:A:112:VAL:O	2.53	0.41
1:C:455:LYS:O	1:C:458:LEU:CB	2.69	0.41
1:A:97:LEU:O	1:A:100:PHE:HB3	2.20	0.41
1:B:206:LEU:O	1:B:210:GLN:HB2	2.20	0.41
1:C:446:ASP:C	1:C:448:ASP:N	2.72	0.41
1:A:44:ASP:O	1:A:45:ASP:C	2.56	0.41
1:C:405:LEU:HA	1:C:405:LEU:HD23	1.85	0.41
1:C:516:HIS:O	1:C:519:LEU:HB3	2.21	0.41
1:A:99:LEU:HD11	1:C:431:CYS:HB2	2.01	0.41
1:A:111:ASP:O	1:A:112:VAL:C	2.59	0.41
1:C:450:GLN:NE2	1:C:453:PHE:N	2.69	0.41
1:B:270:LYS:O	1:B:270:LYS:HG3	2.21	0.41
1:C:406:LEU:O	1:C:410:GLN:HB2	2.22	0.41
1:A:62:PHE:CE1	1:C:412:VAL:HG23	2.55	0.40
1:A:26:GLN:O	1:A:30:ARG:HG3	2.22	0.40
1:B:247:TYR:OH	1:B:258:LEU:HD21	2.22	0.40
1:C:487:LYS:CE	1:C:524:GLY:HA3	2.51	0.40
1:A:52:PHE:O	1:A:56:PRO:HD2	2.18	0.40
1:B:250:GLN:N	2:B:68:HOH:O	2.54	0.40
1:A:50:GLN:HG3	1:A:50:GLN:H	1.70	0.40
1:A:86:VAL:HA	1:C:402:LYS:CE	2.52	0.40
1:A:87:LYS:CE	1:A:124:GLY:HA3	2.51	0.40
1:B:319:LEU:CD1	1:B:319:LEU:C	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	118/135 (87%)	102 (86%)	15 (13%)	1 (1%)	19 29
1	B	118/135 (87%)	104 (88%)	11 (9%)	3 (2%)	5 6
1	C	111/135 (82%)	104 (94%)	6 (5%)	1 (1%)	17 25
All	All	347/405 (86%)	310 (89%)	32 (9%)	5 (1%)	11 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	THR
1	A	39	LEU
1	B	239	LEU
1	B	286	VAL
1	C	439	LEU

5.3.2 Protein sidechains

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	112/118 (95%)	87 (78%)	25 (22%)	1 1
1	B	112/118 (95%)	88 (79%)	24 (21%)	1 1
1	C	106/118 (90%)	85 (80%)	21 (20%)	1 1
All	All	330/354 (93%)	260 (79%)	70 (21%)	1 1

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	LEU
1	A	8	LEU
1	A	12	VAL
1	A	19	VAL
1	A	25	ARG
1	A	32	LEU
1	A	37	SER
1	A	39	LEU
1	A	41	ILE
1	A	44	ASP
1	A	49	ASP
1	A	50	GLN
1	A	58	LEU
1	A	60	ASP
1	A	66	SER
1	A	70	LYS
1	A	72	LEU
1	A	87	LYS
1	A	98	THR
1	A	99	LEU
1	A	111	ASP
1	A	114	ARG
1	A	119	LEU
1	A	121	LYS
1	B	202	LYS
1	B	205	LEU
1	B	208	LEU
1	B	212	VAL
1	B	215	GLU
1	B	232	LEU
1	B	239	LEU
1	B	243	GLU
1	B	249	ASP
1	B	254	LEU
1	B	257	MET
1	B	258	LEU
1	B	273	ASP
1	B	274	LEU
1	B	282	PRO
1	B	283	LYS
1	B	285	ASP
1	B	287	LYS

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Mol	Chain	Res	Type
1	B	288	SER
1	B	298	THR
1	B	301	ILE
1	B	311	ASP
1	B	319	LEU
1	B	321	LYS
1	C	405	LEU
1	C	408	LEU
1	C	415	GLU
1	C	418	LYS
1	C	419	VAL
1	C	422	GLU
1	C	425	ARG
1	C	432	LEU
1	C	435	GLU
1	C	439	LEU
1	C	449	ASP
1	C	450	GLN
1	C	454	LEU
1	C	458	LEU
1	C	460	ASP
1	C	466	SER
1	C	498	THR
1	C	499	LEU
1	C	511	ASP
1	C	519	LEU
1	C	521	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	36	GLN
1	A	71	GLN
1	A	91	GLN
1	B	236	GLN
1	B	271	GLN
1	B	291	GLN
1	C	436	GLN
1	C	450	GLN
1	C	491	GLN

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

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	122/135 (90%)	0.79	14 (11%) 4 4	18, 37, 94, 173	0
1	B	122/135 (90%)	0.77	12 (9%) 7 7	18, 39, 102, 171	0
1	C	115/135 (85%)	0.66	6 (5%) 27 26	19, 37, 72, 138	0
All	All	359/405 (88%)	0.74	32 (8%) 9 9	18, 37, 94, 173	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	439	LEU	13.6
1	A	73	ASP	10.4
1	B	274	LEU	8.5
1	A	39	LEU	8.0
1	A	82	PRO	7.5
1	B	283	LYS	7.4
1	B	272	LEU	5.8
1	C	440	LEU	5.6
1	B	239	LEU	5.6
1	A	45	ASP	5.5
1	C	447	TYR	5.0
1	B	247	TYR	4.7
1	A	74	LEU	4.2
1	A	47	TYR	4.0
1	B	284	GLY	4.0
1	C	445	ASP	3.8
1	A	83	LYS	3.7
1	B	245	ASP	3.5
1	C	471	GLN	3.4
1	A	62	PHE	3.3
1	A	1	MET	3.3
1	B	240	LEU	3.0
1	A	40	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	46	ASP	2.8
1	B	282	PRO	2.7
1	B	273	ASP	2.6
1	B	246	ASP	2.5
1	A	38	THR	2.4
1	A	119	LEU	2.3
1	A	71	GLN	2.3
1	C	446	ASP	2.2
1	B	287	LYS	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.