



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 03:20 PM GMT

PDB ID : 4M0D
Title : Crystal structure of MurQ from H.influenzae in apo form
Authors : Hazra, S.; Blanchard, J.
Deposited on : 2013-08-01
Resolution : 2.58 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

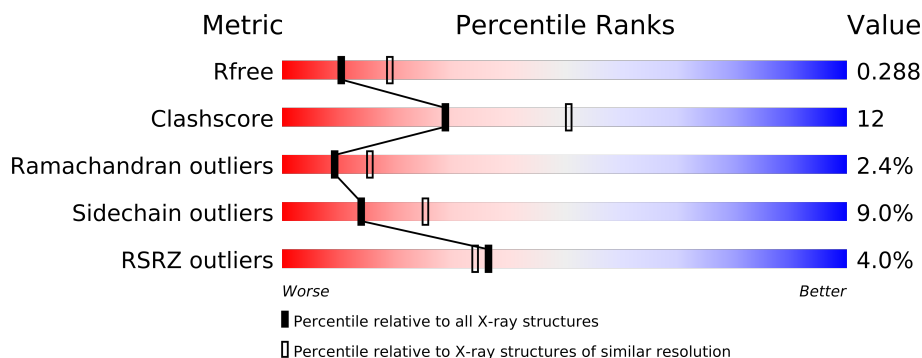
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.58 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}	66092	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	303	
1	B	303	
1	C	303	
1	D	303	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9133 atoms, of which 0 are hydrogen and 0 are deuterium.

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 N-acetylmuramic acid 6-phosphate etherase.

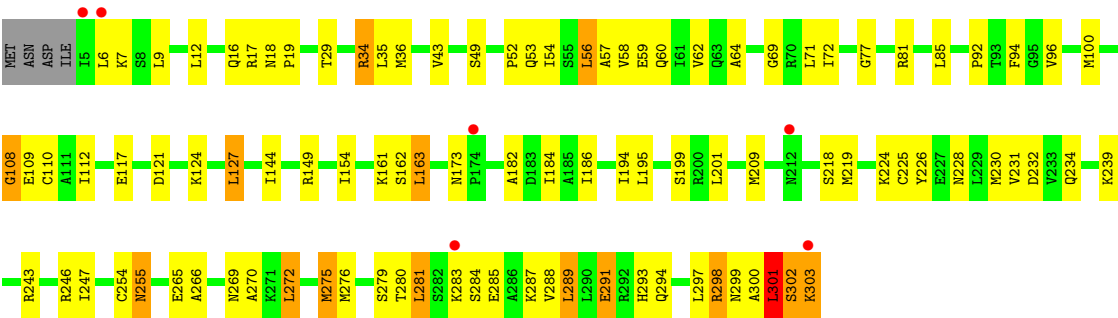
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	1	0
			2234	1394	386	439	15			
1	B	291	Total	C	N	O	S	0	0	0
			2170	1353	375	427	15			
1	C	297	Total	C	N	O	S	0	1	0
			2213	1382	380	436	15			
1	D	299	Total	C	N	O	S	0	0	0
			2233	1393	387	438	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	73	Total	O	0	0
			73	73		
2	C	69	Total	O	0	0
			69	69		
2	D	52	Total	O	0	0
			52	52		

● Molecule 1: N-acetylmuramic acid 6-phosphate etherase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.13Å 111.65Å 134.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.56 – 2.58 32.56 – 2.58	Depositor EDS
% Data completeness (in resolution range)	92.8 (32.56-2.58) 92.8 (32.56-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.183 , 0.286 0.186 , 0.288	Depositor DCC
R_{free} test set	2001 reflections (5.84%)	DCC
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 34270 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9133	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.41	0/2252	0.64	1/3043 (0.0%)
1	B	0.41	0/2188	0.63	0/2958
1	C	0.41	0/2231	0.65	0/3017
1	D	0.39	0/2251	0.60	1/3040 (0.0%)
All	All	0.40	0/8922	0.63	2/12058 (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	A	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	LEU	CA-CB-CG	5.81	128.66	115.30
1	D	301	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	CYS	Peptide
1	C	136	SER	Peptide
1	C	285	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2234	0	2328	59	0
1	B	2170	0	2252	46	0
1	C	2213	0	2299	75	0
1	D	2233	0	2332	70	0
2	A	89	0	0	5	0
2	B	73	0	0	2	0
2	C	69	0	0	11	0
2	D	52	0	0	7	0
All	All	9133	0	9211	224	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (224) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:77:GLY:O	2:C:450:HOH:O	1.78	0.99
1:C:87:ALA:O	2:C:445:HOH:O	1.86	0.92
1:B:39:GLU:HB3	1:B:202:LYS:HE3	1.53	0.91
1:D:254:CYS:SG	2:D:436:HOH:O	2.30	0.90
1:C:89:GLU:O	2:C:468:HOH:O	1.92	0.87
2:A:433:HOH:O	1:D:230:MET:SD	2.38	0.80
1:D:231:VAL:O	2:D:412:HOH:O	2.01	0.79
1:C:93:THR:N	2:C:468:HOH:O	2.10	0.77
2:B:456:HOH:O	1:C:230:MET:SD	2.42	0.75
1:D:7:LYS:HB3	1:D:9:LEU:HG	1.69	0.75
1:A:252:THR:O	1:A:254:CYS:N	2.20	0.74
1:A:26:ARG:HG3	1:D:298:ARG:HH22	1.52	0.74
1:C:272:LEU:HD13	1:C:285:GLU:HB3	1.71	0.73
1:C:78:THR:O	2:C:449:HOH:O	2.07	0.72
1:C:283:LYS:N	1:C:284:SER:HB3	2.04	0.72
1:A:9:LEU:HB3	1:A:15:GLU:HG3	1.73	0.70
1:A:23:ASP:OD1	1:A:23:ASP:N	2.24	0.70
1:D:36:MET:HG2	1:D:194:ILE:HD13	1.73	0.69
1:B:252:THR:O	1:B:254:CYS:N	2.25	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:275:MET:HE1	1:B:297:LEU:HD13	1.74	0.68
1:A:54:ILE:HD13	1:A:213:MET:HE1	1.74	0.68
1:A:148:GLY:N	2:A:458:HOH:O	2.25	0.68
1:B:280:THR:OG1	1:B:281:LEU:N	2.28	0.67
1:D:108:GLY:O	1:D:110:CYS:N	2.24	0.67
1:A:59:GLU:OE2	2:A:449:HOH:O	2.15	0.65
1:D:161:LYS:O	1:D:163:LEU:N	2.30	0.64
1:B:252:THR:OG1	1:B:252:THR:O	2.11	0.64
1:D:276:MET:SD	1:D:283:LYS:NZ	2.70	0.64
1:D:218:SER:O	2:D:423:HOH:O	2.15	0.63
1:B:53:GLN:NE2	2:B:405:HOH:O	2.31	0.62
1:D:92:PRO:HA	1:D:234:GLN:HG3	1.81	0.62
1:A:26:ARG:HG3	1:D:298:ARG:NH2	2.14	0.61
1:D:275:MET:HE1	1:D:289:LEU:HD12	1.83	0.60
1:C:59:GLU:OE2	2:C:461:HOH:O	2.16	0.60
1:C:212:ASN:O	1:C:216:THR:OG1	2.14	0.60
1:A:39:GLU:HG3	1:A:202:LYS:HD3	1.82	0.60
1:D:299:ASN:O	1:D:303:LYS:HB2	2.02	0.59
1:A:99:GLU:OE2	1:A:102:LYS:NZ	2.33	0.59
1:B:74:ILE:HG12	1:B:141:LEU:HD11	1.85	0.59
1:D:7:LYS:HA	1:D:9:LEU:H	1.67	0.58
1:A:267:ASP:O	1:A:269:ASN:N	2.36	0.58
1:A:161:LYS:NZ	2:A:470:HOH:O	2.36	0.58
1:A:6:LEU:HD12	1:D:239:LYS:HA	1.85	0.58
1:A:237:ASN:HB2	1:D:121:ASP:OD1	2.03	0.58
1:C:25:ASP:N	1:C:25:ASP:OD1	2.34	0.57
1:C:135:PHE:HD1	1:C:163:LEU:HD12	1.70	0.57
1:C:279:SER:HB2	1:C:281:LEU:HD22	1.87	0.56
1:C:82:LEU:HG	2:C:449:HOH:O	2.05	0.56
1:A:252:THR:OG1	1:A:254:CYS:HB3	2.06	0.56
1:B:149:ARG:HA	1:B:154:ILE:HD11	1.86	0.56
1:A:94:PHE:CD2	1:A:219:MET:HG3	2.42	0.55
1:C:283:LYS:H	1:C:284:SER:HB3	1.69	0.55
1:B:45:LEU:HD23	1:C:41:LYS:HE2	1.88	0.55
1:A:10:SER:HA	1:D:246:ARG:NH2	2.23	0.54
1:A:15:GLU:O	1:D:246:ARG:NH1	2.39	0.54
1:B:99:GLU:OE2	1:B:102:LYS:NZ	2.20	0.54
1:A:268:GLN:NE2	1:A:268:GLN:O	2.42	0.53
1:B:298:ARG:HG3	1:C:26:ARG:HH11	1.72	0.53
1:C:58:VAL:O	1:C:62:VAL:HG23	2.07	0.53
1:D:149:ARG:NH1	2:D:405:HOH:O	2.41	0.53
1:C:254:CYS:SG	1:C:259:ALA:HB2	2.48	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:192:PRO:O	1:B:202:LYS:NZ	2.39	0.53
1:D:232:ASP:N	2:D:433:HOH:O	2.17	0.53
1:C:82:LEU:N	2:C:449:HOH:O	2.42	0.53
1:B:65:PHE:HB3	1:B:222:LEU:HD11	1.92	0.52
1:C:24:ILE:HD12	1:C:35:LEU:HD23	1.90	0.52
1:D:56:LEU:O	1:D:60:GLN:HG2	2.08	0.52
1:A:6:LEU:HD21	1:A:149:ARG:NH1	2.24	0.52
1:A:74:ILE:HG13	1:A:143:GLY:HA2	1.90	0.52
1:B:261:GLN:O	1:B:264:LEU:HB2	2.11	0.51
1:B:17:ARG:NH2	1:C:228:ASN:OD1	2.41	0.51
1:D:34:ARG:HB3	1:D:34:ARG:HH11	1.76	0.51
1:C:52:PRO:O	1:C:55:SER:HB3	2.11	0.51
1:C:114:HIS:ND1	1:C:115:PRO:O	2.41	0.51
1:B:24:ILE:HD12	1:C:220:ILE:HD13	1.92	0.51
1:A:147:SER:HA	1:A:173:ASN:ND2	2.26	0.51
1:D:281:LEU:HB3	1:D:285:GLU:HG3	1.93	0.51
1:B:21:SER:O	1:C:228:ASN:HB3	2.11	0.50
1:C:47:ILE:HD11	1:C:206:ALA:HB1	1.93	0.50
1:A:238:GLU:HG2	1:D:121:ASP:OD2	2.13	0.49
1:B:91:PRO:HG2	1:B:98:THR:HG22	1.95	0.49
1:D:58:VAL:O	1:D:62:VAL:HG23	2.12	0.49
1:B:195:LEU:HB3	1:B:198:SER:HB2	1.95	0.49
1:B:262:THR:HG21	1:B:277:ILE:HG13	1.93	0.49
1:D:300:ALA:O	1:D:301:LEU:HB3	2.12	0.49
1:C:288:VAL:O	1:C:289:LEU:HB2	2.13	0.49
1:C:250:GLN:OE1	2:C:416:HOH:O	2.20	0.49
1:A:252:THR:O	1:A:252:THR:OG1	2.29	0.48
1:B:94:PHE:CD2	1:B:219:MET:HG3	2.48	0.48
1:B:92:PRO:HA	1:B:234:GLN:HB2	1.96	0.48
1:B:89:GLU:OE2	1:C:78:THR:OG1	2.20	0.48
1:D:12:LEU:HB3	1:D:173:ASN:ND2	2.29	0.48
1:A:265:GLU:O	1:A:283:LYS:HD2	2.13	0.47
1:D:230:MET:CE	1:D:243:ARG:HH11	2.27	0.47
1:B:256:LYS:HG3	1:C:7:LYS:HE2	1.96	0.47
1:A:126:VAL:HB	1:A:152:TYR:CE1	2.49	0.47
1:C:285:GLU:HA	1:C:290:LEU:HB2	1.97	0.47
1:D:96:VAL:HB	1:D:100:MET:HE3	1.97	0.47
1:B:298:ARG:N	1:B:298:ARG:HH11	2.12	0.47
1:D:182:ALA:O	2:D:431:HOH:O	2.21	0.47
1:C:85:LEU:HD13	2:C:417:HOH:O	2.15	0.47
1:B:54:ILE:HG12	1:B:186:ILE:HD13	1.97	0.47
1:C:5:ILE:HG23	1:C:6:LEU:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:39:GLU:HG3	1:C:194:ILE:HD13	1.97	0.46
1:A:198:SER:HB3	1:A:201:LEU:HD12	1.97	0.46
1:A:147:SER:HA	1:A:173:ASN:HD22	1.79	0.46
1:A:59:GLU:HG3	1:D:29:THR:HG21	1.98	0.46
1:C:5:ILE:HG12	1:C:6:LEU:H	1.80	0.46
1:C:5:ILE:HG12	1:C:6:LEU:N	2.29	0.46
1:A:29:THR:HG21	1:D:59:GLU:HG3	1.98	0.46
1:B:245:VAL:O	1:B:249:MET:HG3	2.16	0.46
1:D:301:LEU:O	1:D:302:SER:HB3	2.15	0.46
1:D:7:LYS:HA	1:D:9:LEU:N	2.31	0.46
1:C:54:ILE:O	1:C:58:VAL:HG23	2.16	0.46
1:A:266:ALA:HA	1:A:283:LYS:HE3	1.98	0.46
1:A:21:SER:O	1:D:228:ASN:HB3	2.16	0.46
1:A:272:LEU:O	1:A:276:MET:HG2	2.16	0.46
1:D:230:MET:HB3	1:D:230:MET:HE3	1.69	0.46
1:B:298:ARG:HD3	1:B:298:ARG:HA	1.52	0.46
1:A:25:ASP:OD1	1:A:26:ARG:NH1	2.49	0.46
1:A:5:ILE:N	1:A:7:LYS:HZ3	2.14	0.46
1:B:89:GLU:OE1	1:C:200:ARG:HD2	2.15	0.45
1:B:231:VAL:O	1:B:270:ALA:HB3	2.17	0.45
1:D:224:LYS:HD3	1:D:232:ASP:OD2	2.15	0.45
1:D:54:ILE:HG13	1:D:186:ILE:HD13	1.97	0.45
1:B:31:GLU:OE1	1:B:34:ARG:NH2	2.47	0.45
1:A:116:VAL:HB	1:A:119:ALA:HB2	1.97	0.45
1:B:154:ILE:HG12	1:B:178:MET:HG3	1.99	0.45
1:C:206:ALA:HA	1:C:209:MET:HE2	1.98	0.45
1:A:225:CYS:HB2	1:A:229:LEU:O	2.16	0.45
1:D:293:HIS:HB3	1:D:299:ASN:HB2	1.99	0.45
1:D:94:PHE:CD2	1:D:219:MET:HG3	2.52	0.45
1:D:291:GLU:HG2	1:D:291:GLU:H	1.58	0.45
1:A:6:LEU:HA	1:A:6:LEU:HD23	1.65	0.44
1:D:149:ARG:HA	1:D:154:ILE:HD11	1.99	0.44
1:C:283:LYS:HB3	1:C:286:ALA:O	2.18	0.44
1:D:266:ALA:HA	1:D:283:LYS:HD3	1.99	0.44
1:C:271:LYS:HG3	1:C:297:LEU:HD22	2.00	0.44
1:C:230:MET:HE3	1:C:230:MET:HB2	1.83	0.44
1:D:52:PRO:HG2	1:D:53:GLN:OE1	2.17	0.44
1:A:219:MET:O	1:A:224:LYS:HB2	2.17	0.44
1:A:5:ILE:HG12	1:A:7:LYS:NZ	2.32	0.44
1:B:246:ARG:HA	1:B:249:MET:HE2	1.98	0.44
1:B:122:ASN:ND2	1:B:124:LYS:HD2	2.33	0.44
1:A:54:ILE:O	1:A:58:VAL:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:226:TYR:HB2	1:D:297:LEU:HD23	2.00	0.44
1:D:231:VAL:O	1:D:232:ASP:HB2	2.18	0.43
1:D:18:ASN:HA	1:D:19:PRO:HD2	1.85	0.43
1:C:262:THR:HG21	1:C:277:ILE:HG13	2.00	0.43
1:A:250:GLN:HB3	1:D:17:ARG:HH11	1.83	0.43
1:A:174:PRO:HD3	1:A:189:ILE:HD12	2.00	0.43
1:C:291:GLU:HA	1:C:292:ARG:HA	1.57	0.43
1:D:124:LYS:HE2	1:D:127:LEU:HD22	2.00	0.43
1:C:209:MET:HB2	1:C:209:MET:HE3	1.51	0.43
1:B:94:PHE:HB3	1:B:224:LYS:HB3	2.00	0.43
1:D:43:VAL:HG12	1:D:209:MET:HE1	2.01	0.43
1:A:147:SER:HB2	1:A:149:ARG:HG3	2.00	0.43
1:C:259:ALA:O	1:C:263:LEU:N	2.35	0.43
1:C:279:SER:OG	1:C:281:LEU:HB2	2.18	0.43
1:B:207:GLN:O	1:B:211:LEU:HG	2.19	0.43
1:A:12:LEU:O	1:A:16:GLN:HG3	2.19	0.43
1:B:200:ARG:HD2	1:C:89:GLU:OE1	2.19	0.43
1:C:247:ILE:HG22	1:C:274:ILE:HD11	2.01	0.43
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.87	0.43
1:B:115:PRO:HG3	1:C:92:PRO:HG3	2.00	0.43
1:D:269:ASN:ND2	1:D:272:LEU:HD23	2.34	0.43
1:A:255:ASN:O	1:A:258:LEU:HB3	2.19	0.43
1:D:285:GLU:HA	1:D:288:VAL:HG22	2.01	0.42
1:A:194:ILE:HA	1:A:194:ILE:HD12	1.65	0.42
1:A:195:LEU:HD22	1:D:230:MET:HB2	2.00	0.42
1:C:287:LYS:HA	1:C:288:VAL:C	2.39	0.42
1:A:263:LEU:HD22	1:A:268:GLN:HA	2.02	0.42
1:A:6:LEU:CD1	1:D:239:LYS:HA	2.49	0.42
1:C:24:ILE:HA	1:C:27:GLN:HG2	2.01	0.42
1:D:279:SER:HB2	1:D:281:LEU:HG	2.01	0.42
1:C:65:PHE:CD2	1:C:222:LEU:HD11	2.53	0.42
1:C:226:TYR:HB3	1:C:231:VAL:HG11	2.01	0.42
1:C:289:LEU:HA	1:C:289:LEU:HD12	1.75	0.42
1:C:94:PHE:HB3	1:C:224:LYS:HB3	2.01	0.42
1:C:258:LEU:HA	1:C:261:GLN:HG2	2.00	0.42
1:B:298:ARG:HG3	1:C:26:ARG:NH1	2.35	0.42
1:C:123:THR:O	1:C:126:VAL:HG12	2.20	0.42
1:A:266:ALA:HA	1:A:283:LYS:CE	2.49	0.42
1:C:194:ILE:HA	1:C:194:ILE:HD12	1.71	0.42
1:B:112:ILE:HG21	1:C:112:ILE:HG21	2.02	0.41
1:D:224:LYS:HD3	1:D:224:LYS:HA	1.85	0.41
1:D:225:CYS:HA	1:D:231:VAL:HG22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:267:ASP:OD1	1:A:268:GLN:N	2.52	0.41
1:B:246:ARG:HH21	1:C:10:SER:HA	1.83	0.41
1:D:265:GLU:HG2	1:D:283:LYS:HE3	2.02	0.41
1:A:144:ILE:HD11	1:A:211:LEU:HD21	2.03	0.41
1:D:92:PRO:HA	1:D:234:GLN:CG	2.49	0.41
1:D:12:LEU:O	1:D:16:GLN:HG3	2.19	0.41
1:C:262:THR:HG22	1:C:273:ALA:HB1	2.01	0.41
1:C:93:THR:HG23	1:C:230:MET:CE	2.50	0.41
1:B:208:LYS:HE2	2:C:406:HOH:O	2.20	0.41
1:C:159:TYR:CE1	1:C:163:LEU:HD21	2.55	0.41
1:C:29:THR:O	1:C:33:VAL:HG22	2.21	0.41
1:D:287:LYS:O	1:D:291:GLU:HG2	2.20	0.41
1:D:7:LYS:CA	1:D:9:LEU:H	2.31	0.41
1:B:88:SER:OG	1:B:89:GLU:HG3	2.21	0.41
1:C:283:LYS:C	1:C:287:LYS:H	2.23	0.41
1:B:275:MET:O	1:B:279:SER:OG	2.37	0.41
1:A:54:ILE:HD13	1:A:213:MET:CE	2.46	0.41
1:D:272:LEU:HD13	1:D:272:LEU:HA	1.83	0.41
1:C:73:TYR:HD1	1:C:142:VAL:HB	1.86	0.41
1:C:195:LEU:HB3	1:C:198:SER:HB2	2.03	0.41
1:A:124:LYS:HB2	2:A:419:HOH:O	2.20	0.41
1:A:6:LEU:HD13	1:A:9:LEU:HD21	2.03	0.41
1:D:57:ALA:HA	1:D:184:ILE:HD13	2.02	0.41
1:D:77:GLY:O	1:D:81:ARG:HG3	2.21	0.41
1:B:297:LEU:O	1:B:297:LEU:HG	2.16	0.40
1:A:111:ALA:HA	1:A:114:HIS:O	2.21	0.40
1:D:199:SER:C	1:D:201:LEU:H	2.24	0.40
1:D:270:ALA:HB3	2:D:433:HOH:O	2.21	0.40
1:C:24:ILE:HG12	1:C:32:ILE:HG12	2.02	0.40
1:C:290:LEU:HA	1:C:290:LEU:HD23	1.89	0.40
1:B:220:ILE:HG22	1:B:221:LEU:HD23	2.04	0.40
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.84	0.40
1:D:64:ALA:O	1:D:69:GLY:N	2.36	0.40
1:D:283:LYS:HE2	1:D:283:LYS:HB2	1.52	0.40
1:C:19:PRO:O	1:C:22:VAL:HG23	2.21	0.40
1:C:242:ALA:O	1:C:246:ARG:HG3	2.22	0.40
1:C:14:THR:O	1:C:197:GLY:HA2	2.22	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	298/303 (98%)	280 (94%)	11 (4%)	7 (2%)	10	17
1	B	289/303 (95%)	269 (93%)	14 (5%)	6 (2%)	11	19
1	C	296/303 (98%)	270 (91%)	19 (6%)	7 (2%)	9	15
1	D	297/303 (98%)	264 (89%)	25 (8%)	8 (3%)	8	12
All	All	1180/1212 (97%)	1083 (92%)	69 (6%)	28 (2%)	9	15

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	253	ASP
1	A	266	ALA
1	A	268	GLN
1	B	253	ASP
1	C	137	LYS
1	C	259	ALA
1	C	289	LEU
1	D	163	LEU
1	A	256	LYS
1	C	282	SER
1	C	284	SER
1	C	288	VAL
1	D	162	SER
1	A	6	LEU
1	B	201	LEU
1	D	117	GLU
1	D	302	SER
1	B	235	ALA
1	B	278	LEU
1	D	301	LEU
1	A	302	SER
1	B	279	SER
1	C	287	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	109	GLU
1	D	255	ASN
1	B	10	SER
1	D	108	GLY

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	248/253 (98%)	224 (90%)	24 (10%)	12	21
1	B	240/253 (95%)	220 (92%)	20 (8%)	16	30
1	C	245/253 (97%)	226 (92%)	19 (8%)	18	34
1	D	248/253 (98%)	223 (90%)	25 (10%)	11	19
All	All	981/1012 (97%)	893 (91%)	88 (9%)	14	25

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	11	THR
1	A	23	ASP
1	A	26	ARG
1	A	71	LEU
1	A	85	LEU
1	A	98	THR
1	A	149	ARG
1	A	180	GLU
1	A	194	ILE
1	A	195	LEU
1	A	252	THR
1	A	254	CYS
1	A	262	THR
1	A	267	ASP
1	A	268	GLN
1	A	274	ILE
1	A	282	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	288	VAL
1	A	289	LEU
1	A	291	GLU
1	A	292	ARG
1	A	298	ARG
1	A	303	LYS
1	B	11	THR
1	B	23	ASP
1	B	24	ILE
1	B	35	LEU
1	B	60	GLN
1	B	71	LEU
1	B	85	LEU
1	B	120	GLU
1	B	195	LEU
1	B	252	THR
1	B	255	ASN
1	B	263	LEU
1	B	275	MET
1	B	280	THR
1	B	283	LYS
1	B	289	LEU
1	B	290	LEU
1	B	291	GLU
1	B	294	GLN
1	B	297	LEU
1	C	6	LEU
1	C	26	ARG
1	C	66	GLN
1	C	67	GLN
1	C	71	LEU
1	C	85	LEU
1	C	120	GLU
1	C	131	GLN
1	C	149	ARG
1	C	194	ILE
1	C	195	LEU
1	C	215	THR
1	C	216	THR
1	C	253	ASP
1	C	264	LEU
1	C	281	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	285	GLU
1	C	289	LEU
1	C	301	LEU
1	D	6	LEU
1	D	34	ARG
1	D	35	LEU
1	D	49	SER
1	D	56	LEU
1	D	71	LEU
1	D	72	ILE
1	D	85	LEU
1	D	112	ILE
1	D	127	LEU
1	D	144	ILE
1	D	195	LEU
1	D	247	ILE
1	D	255	ASN
1	D	272	LEU
1	D	275	MET
1	D	280	THR
1	D	281	LEU
1	D	284	SER
1	D	289	LEU
1	D	291	GLU
1	D	294	GLN
1	D	298	ARG
1	D	301	LEU
1	D	303	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	250	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/303 (98%)	0.23	15 (5%) 28 25	13, 24, 56, 74	0
1	B	291/303 (96%)	0.29	19 (6%) 18 16	12, 25, 54, 71	0
1	C	297/303 (98%)	0.12	8 (2%) 52 50	13, 27, 46, 82	0
1	D	299/303 (98%)	0.10	6 (2%) 62 61	18, 31, 50, 63	0
All	All	1186/1212 (97%)	0.18	48 (4%) 36 34	12, 28, 52, 82	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	288	VAL	11.7
1	C	286	ALA	9.2
1	B	281	LEU	5.7
1	A	6	LEU	4.9
1	B	10	SER	3.8
1	B	292	ARG	3.7
1	B	286	ALA	3.6
1	C	285	GLU	3.4
1	A	264	LEU	3.4
1	C	289	LEU	3.3
1	A	5	ILE	3.3
1	A	255	ASN	3.0
1	B	289	LEU	3.0
1	C	9	LEU	2.7
1	D	5	ILE	2.7
1	A	268	GLN	2.7
1	B	205	THR	2.7
1	A	261	GLN	2.7
1	B	282	SER	2.6
1	A	288	VAL	2.6
1	D	283	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	264	LEU	2.5
1	B	287	LYS	2.4
1	A	303	LYS	2.4
1	B	293	HIS	2.4
1	D	174	PRO	2.4
1	D	212	ASN	2.4
1	A	85	LEU	2.4
1	B	278	LEU	2.4
1	D	6	LEU	2.4
1	A	267	ASP	2.3
1	B	288	VAL	2.3
1	B	204	GLY	2.3
1	D	303	LYS	2.3
1	A	245	VAL	2.3
1	A	212	ASN	2.3
1	B	265	GLU	2.3
1	C	264	LEU	2.2
1	A	283	LYS	2.2
1	B	210	VAL	2.2
1	B	284	SER	2.2
1	A	277	ILE	2.2
1	A	78	THR	2.1
1	B	291	GLU	2.1
1	C	256	LYS	2.1
1	B	203	SER	2.0
1	B	9	LEU	2.0
1	C	291	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.