Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 10:49 AM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

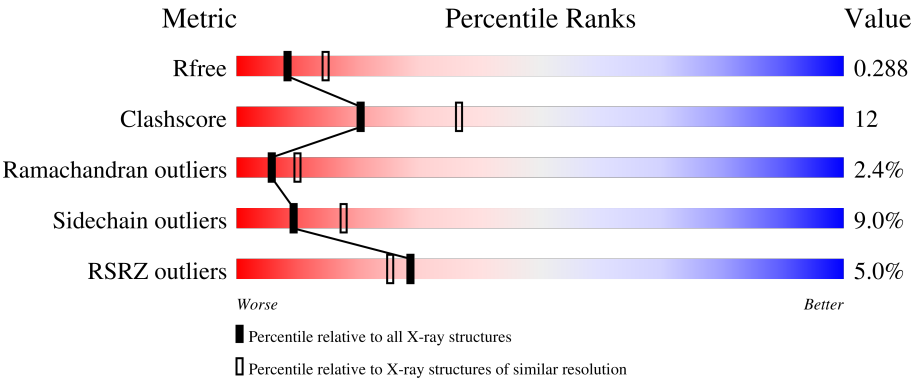
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.58 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	6% 71% 23%
1	B	303	8% 70% 24%
1	C	303	3% 65% 29%
1	D	303	2% 66% 28% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9133 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 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			

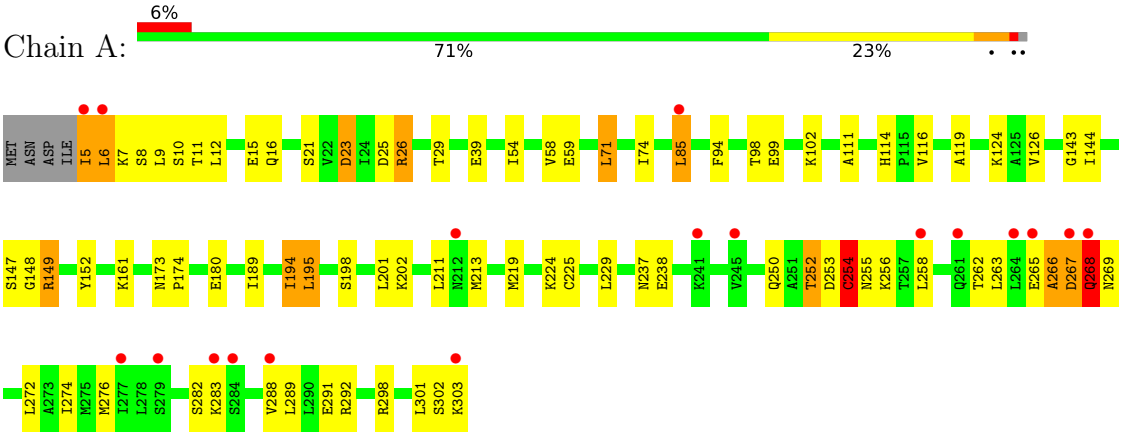
- Molecule 2 is water.

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		

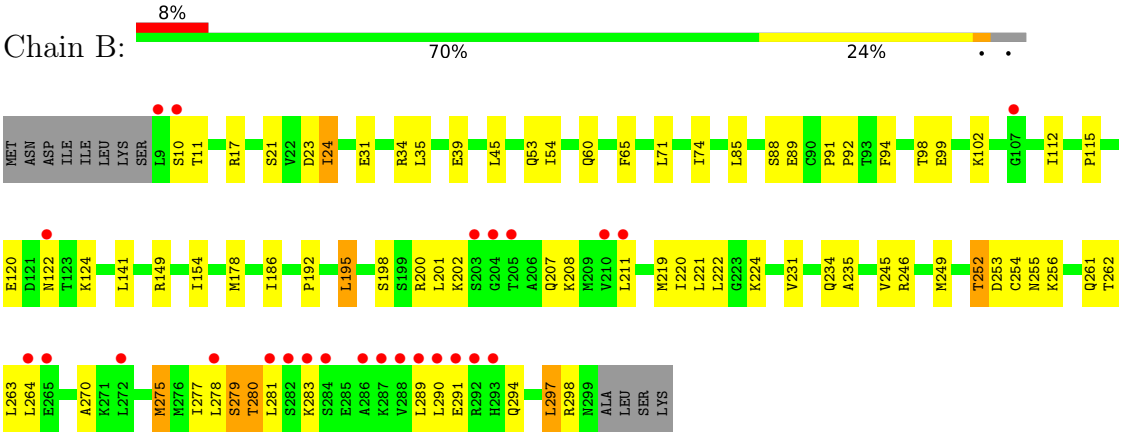
3 Residue-property plots (i)

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.

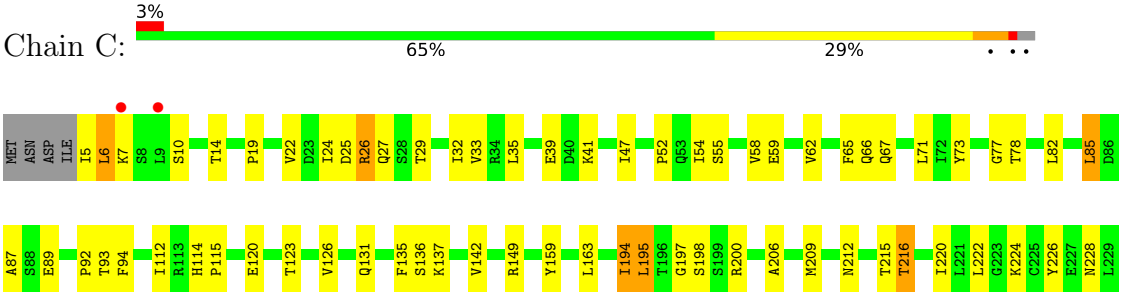
• Molecule 1: N-acetylmuramic acid 6-phosphate etherase

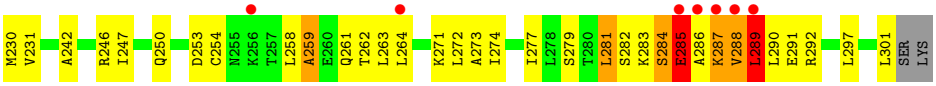


• Molecule 1: N-acetylmuramic acid 6-phosphate etherase



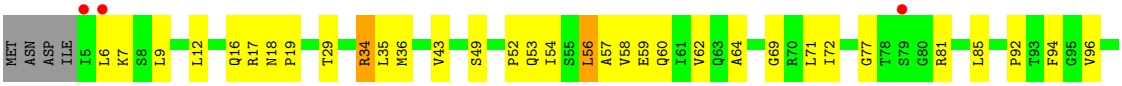
• Molecule 1: N-acetylmuramic acid 6-phosphate etherase

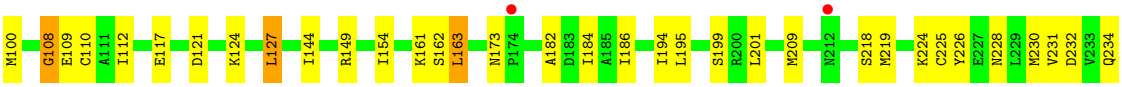


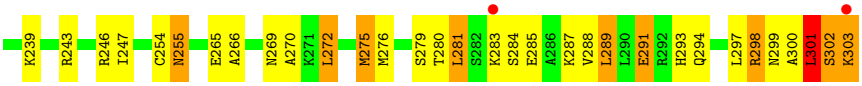


• Molecule 1: N-acetylmuramic acid 6-phosphate etherase

Chain D:







4 Data and refinement statistics (i)

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) 92.9 (32.56-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.57Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.183 , 0.286 0.186 , 0.288	Depositor DCC
R_{free} test set	2000 reflections (5.84%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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	0.41	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(^{o})	Ideal(^{o})
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 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	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

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 12.

All (224) 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: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:26:ARG:HG3	1:D:298:ARG:HH22	1.52	0.74
1:A:252:THR:O	1:A:254:CYS:N	2.20	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:N	1:A:23:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:O	1:B:252:THR:OG1	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:OD1	1:C:25:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:CYS:SG	1:C:259:ALA:HB2	2.48	0.53
1:B:192:PRO:O	1:B:202:LYS:NZ	2.39	0.53
1:C:82:LEU:N	2:C:449:HOH:O	2.42	0.53
1:D:232:ASP:N	2:D:433:HOH:O	2.17	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:HH11	1:D:34:ARG:HB3	1.76	0.51
1:B:24:ILE:HD12	1:C:220:ILE:HD13	1.92	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: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:C:85:LEU:HD13	2:C:417:HOH:O	2.15	0.47
1:D:182:ALA:O	2:D:431:HOH:O	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ILE:HG12	1:B:186:ILE:HD13	1.97	0.47
1:A:198:SER:HB3	1:A:201:LEU:HD12	1.97	0.46
1:C:5:ILE:HG23	1:C:6:LEU:H	1.80	0.46
1:C:39:GLU:HG3	1:C:194:ILE:HD13	1.97	0.46
1:A:59:GLU:HG3	1:D:29:THR:HG21	1.98	0.46
1:A:147:SER:HA	1:A:173:ASN:HD22	1.79	0.46
1:C:5:ILE:HG12	1:C:6:LEU:H	1.80	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:C:5:ILE:HG12	1:C:6:LEU:N	2.29	0.46
1:D:301:LEU:O	1:D:302:SER:HB3	2.15	0.46
1:A:21:SER:O	1:D:228:ASN:HB3	2.16	0.46
1:A:266:ALA:HA	1:A:283:LYS:HE3	1.98	0.46
1:A:272:LEU:O	1:A:276:MET:HG2	2.16	0.46
1:C:54:ILE:O	1:C:58:VAL:HG23	2.16	0.46
1:D:7:LYS:HA	1:D:9:LEU:N	2.31	0.46
1:B:298:ARG:HD3	1:B:298:ARG:HA	1.52	0.46
1:D:230:MET:HE3	1:D:230:MET:HB3	1.69	0.46
1:A:5:ILE:N	1:A:7:LYS:HZ3	2.14	0.46
1:A:25:ASP:OD1	1:A:26:ARG:NH1	2.49	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:A:116:VAL:HB	1:A:119:ALA:HB2	1.97	0.45
1:B:31:GLU:OE1	1:B:34:ARG:NH2	2.47	0.45
1:A:225:CYS:HB2	1:A:229:LEU:O	2.16	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:D:94:PHE:CD2	1:D:219:MET:HG3	2.52	0.45
1:D:293:HIS:HB3	1:D:299:ASN:HB2	1.99	0.45
1:D:291:GLU:H	1:D:291:GLU:HG2	1.58	0.45
1:A:6:LEU:HD23	1:A:6:LEU:HA	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:HB2	1:C:230:MET:HE3	1.83	0.44
1:D:52:PRO:HG2	1:D:53:GLN:OE1	2.17	0.44
1:A:5:ILE:HG12	1:A:7:LYS:NZ	2.32	0.44
1:A:219:MET:O	1:A:224:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASN:ND2	1:B:124:LYS:HD2	2.33	0.44
1:B:246:ARG:HA	1:B:249:MET:HE2	1.98	0.44
1:A:54:ILE:O	1:A:58:VAL:HG23	2.18	0.44
1:D:226:TYR:HB2	1:D:297:LEU:HD23	2.00	0.44
1:D:18:ASN:HA	1:D:19:PRO:HD2	1.85	0.43
1:D:231:VAL:O	1:D:232:ASP:HB2	2.18	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:B:94:PHE:HB3	1:B:224:LYS:HB3	2.00	0.43
1:C:209:MET:HB2	1:C:209:MET:HE3	1.51	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:A:12:LEU:O	1:A:16:GLN:HG3	2.19	0.43
1:B:207:GLN:O	1:B:211:LEU:HG	2.19	0.43
1:C:279:SER:OG	1:C:281:LEU:HB2	2.18	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: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: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:A:194:ILE:HA	1:A:194:ILE:HD12	1.65	0.42
1:D:285:GLU:HA	1:D:288:VAL:HG22	2.01	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: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:D:279:SER:HB2	1:D:281:LEU:HG	2.01	0.42
1:C:94:PHE:HB3	1:C:224:LYS:HB3	2.01	0.42
1:C:289:LEU:HD12	1:C:289:LEU:HA	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ILE:HD12	1:C:194:ILE:HA	1.71	0.42
1:B:112:ILE:HG21	1:C:112:ILE:HG21	2.02	0.41
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: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
1:A:144:ILE:HD11	1:A:211:LEU:HD21	2.03	0.41
1:D:265:GLU:HG2	1:D:283:LYS:HE3	2.02	0.41
1:C:262:THR:HG22	1:C:273:ALA:HB1	2.01	0.41
1:D:12:LEU:O	1:D:16:GLN:HG3	2.19	0.41
1:D:92:PRO:HA	1:D:234:GLN:CG	2.49	0.41
1:B:208:LYS:HE2	2:C:406:HOH:O	2.20	0.41
1:C:93:THR:HG23	1:C:230:MET:CE	2.50	0.41
1:C:29:THR:O	1:C:33:VAL:HG22	2.21	0.41
1:C:159:TYR:CE1	1:C:163:LEU:HD21	2.55	0.41
1:D:287:LYS:O	1:D:291:GLU:HG2	2.20	0.41
1:A:54:ILE:HD13	1:A:213:MET:CE	2.46	0.41
1:A:124:LYS:HB2	2:A:419:HOH:O	2.20	0.41
1:B:88:SER:OG	1:B:89:GLU:HG3	2.21	0.41
1:B:275:MET:O	1:B:279:SER:OG	2.37	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:C:283:LYS:C	1:C:287:LYS:H	2.23	0.41
1:D:7:LYS:CA	1:D:9:LEU:H	2.31	0.41
1:D:272:LEU:HA	1:D:272:LEU:HD13	1.83	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:A:111:ALA:HA	1:A:114:HIS:O	2.21	0.40
1:B:297:LEU:O	1:B:297:LEU:HG	2.16	0.40
1:D:199:SER:C	1:D:201:LEU:H	2.24	0.40
1:C:24:ILE:HG12	1:C:32:ILE:HG12	2.02	0.40
1:D:270:ALA:HB3	2:D:433:HOH:O	2.21	0.40
1:B:220:ILE:HG22	1:B:221:LEU:HD23	2.04	0.40
1:C:290:LEU:HD23	1:C:290:LEU:HA	1.89	0.40
1:A:301:LEU:HA	1:A:301:LEU:HD23	1.84	0.40
1:D:64:ALA:O	1:D:69:GLY:N	2.36	0.40
1:C:14:THR:O	1:C:197:GLY:HA2	2.22	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:D:283:LYS:HB2	1:D:283:LYS:HE2	1.52	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	298/303 (98%)	280 (94%)	11 (4%)	7 (2%)	6 11
1	B	289/303 (95%)	269 (93%)	14 (5%)	6 (2%)	7 12
1	C	296/303 (98%)	270 (91%)	19 (6%)	7 (2%)	6 10
1	D	297/303 (98%)	264 (89%)	25 (8%)	8 (3%)	5 8
All	All	1180/1212 (97%)	1083 (92%)	69 (6%)	28 (2%)	6 10

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

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Mol	Chain	Res	Type
1	D	301	LEU
1	A	302	SER
1	B	279	SER
1	C	287	LYS
1	D	109	GLU
1	D	255	ASN
1	B	10	SER
1	D	108	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	248/253 (98%)	224 (90%)	24 (10%)	8 15
1	B	240/253 (95%)	220 (92%)	20 (8%)	11 21
1	C	245/253 (97%)	226 (92%)	19 (8%)	12 23
1	D	248/253 (98%)	223 (90%)	25 (10%)	7 13
All	All	981/1012 (97%)	893 (91%)	88 (9%)	9 17

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

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Mol	Chain	Res	Type
1	A	262	THR
1	A	267	ASP
1	A	268	GLN
1	A	274	ILE
1	A	282	SER
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

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Mol	Chain	Res	Type
1	C	215	THR
1	C	216	THR
1	C	253	ASP
1	C	264	LEU
1	C	281	LEU
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

Sometimes 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 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	299/303 (98%)	0.20	18 (6%) 21 18	13, 24, 56, 74	0
1	B	291/303 (96%)	0.25	25 (8%) 10 8	12, 25, 54, 71	0
1	C	297/303 (98%)	0.06	9 (3%) 50 46	13, 27, 46, 82	0
1	D	299/303 (98%)	0.05	7 (2%) 60 57	18, 31, 50, 63	0
All	All	1186/1212 (97%)	0.14	59 (4%) 28 25	12, 28, 52, 82	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	288	VAL	11.5
1	C	286	ALA	9.4
1	A	6	LEU	5.6
1	B	281	LEU	5.0
1	A	5	ILE	4.5
1	B	292	ARG	4.2
1	B	286	ALA	4.2
1	A	268	GLN	3.6
1	B	10	SER	3.6
1	D	5	ILE	3.1
1	C	289	LEU	3.0
1	C	285	GLU	3.0
1	A	264	LEU	3.0
1	D	303	LYS	2.9
1	B	291	GLU	2.8
1	B	288	VAL	2.7
1	B	278	LEU	2.7
1	A	277	ILE	2.7
1	D	6	LEU	2.7
1	A	279	SER	2.6
1	B	282	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	9	LEU	2.6
1	C	9	LEU	2.6
1	B	293	HIS	2.6
1	B	205	THR	2.5
1	C	256	LYS	2.5
1	A	283	LYS	2.5
1	A	261	GLN	2.5
1	B	211	LEU	2.4
1	C	264	LEU	2.4
1	A	212	ASN	2.4
1	A	85	LEU	2.4
1	B	265	GLU	2.4
1	B	210	VAL	2.4
1	B	289	LEU	2.4
1	A	288	VAL	2.3
1	A	267	ASP	2.3
1	B	107	GLY	2.3
1	B	204	GLY	2.3
1	D	79	SER	2.3
1	A	258	LEU	2.3
1	B	290	LEU	2.2
1	A	241	LYS	2.2
1	B	264	LEU	2.2
1	D	174	PRO	2.2
1	B	287	LYS	2.2
1	A	284	SER	2.1
1	B	283	LYS	2.1
1	C	7	LYS	2.1
1	B	122	ASN	2.1
1	C	287	LYS	2.1
1	B	284	SER	2.0
1	B	272	LEU	2.0
1	A	245	VAL	2.0
1	A	265	GLU	2.0
1	A	303	LYS	2.0
1	B	203	SER	2.0
1	D	212	ASN	2.0
1	D	283	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.