Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2024 – 12:58 PM JST

PDB ID	:	8I37
Title	:	Helicobacter pylori G6PDH
Authors	:	Zhou, N.; Gao, L.Z.
Deposited on	:	2023-01-16
Resolution	:	2.75 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:

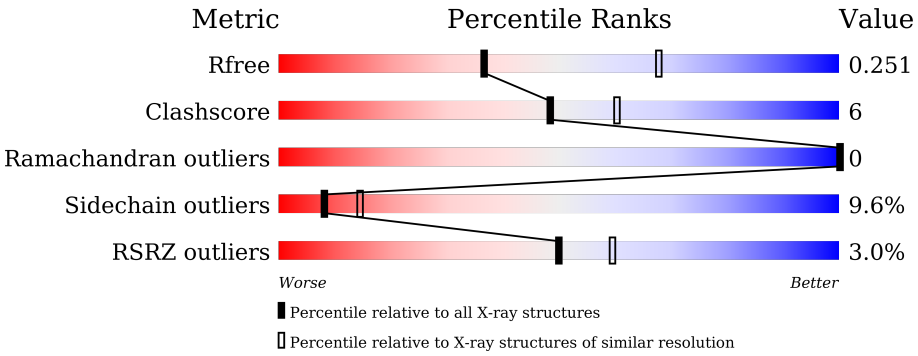
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	428	5% 84% 14%
1	B	428	2% 81% 15%
1	C	428	4% 76% 21%
1	D	428	% 84% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14155 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 Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3522	2281	584	649	8			
1	B	428	Total	C	N	O	S	0	0	0
			3522	2281	584	649	8			
1	C	428	Total	C	N	O	S	0	0	0
			3522	2281	584	649	8			
1	D	428	Total	C	N	O	S	0	0	0
			3522	2281	584	649	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A1U9ITQ5
A	-1	GLU	-	expression tag	UNP A0A1U9ITQ5
A	0	PHE	-	expression tag	UNP A0A1U9ITQ5
B	-2	SER	-	expression tag	UNP A0A1U9ITQ5
B	-1	GLU	-	expression tag	UNP A0A1U9ITQ5
B	0	PHE	-	expression tag	UNP A0A1U9ITQ5
C	-2	SER	-	expression tag	UNP A0A1U9ITQ5
C	-1	GLU	-	expression tag	UNP A0A1U9ITQ5
C	0	PHE	-	expression tag	UNP A0A1U9ITQ5
D	-2	SER	-	expression tag	UNP A0A1U9ITQ5
D	-1	GLU	-	expression tag	UNP A0A1U9ITQ5
D	0	PHE	-	expression tag	UNP A0A1U9ITQ5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	18	Total	O	0	0
			18	18		

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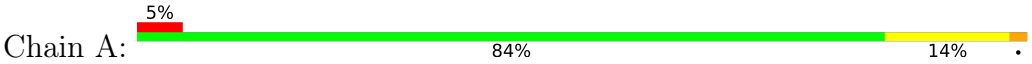
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	17	Total O 17 17	0	0
2	D	18	Total O 18 18	0	0

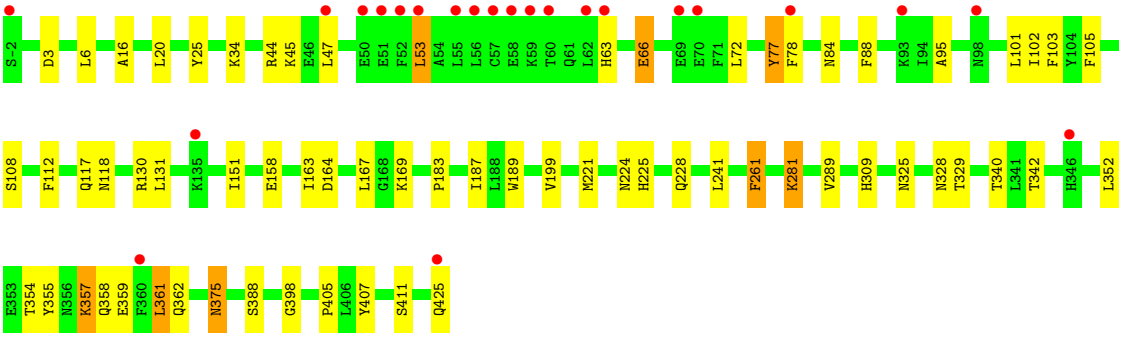
3 Residue-property plots (i)

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: Glucose-6-phosphate 1-dehydrogenase

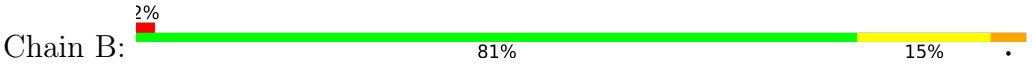
Chain A:

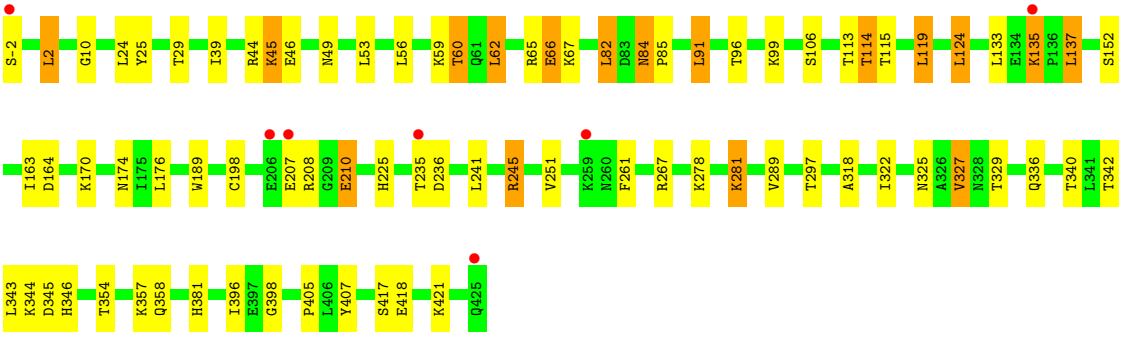




• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

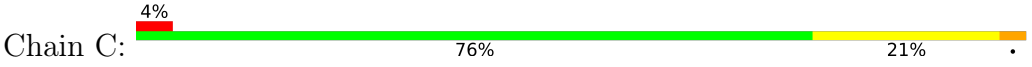
Chain B:

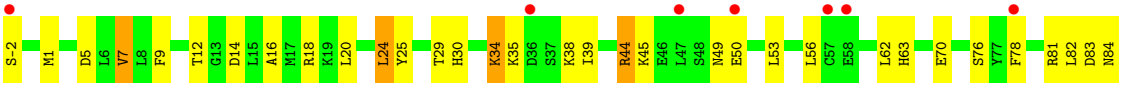


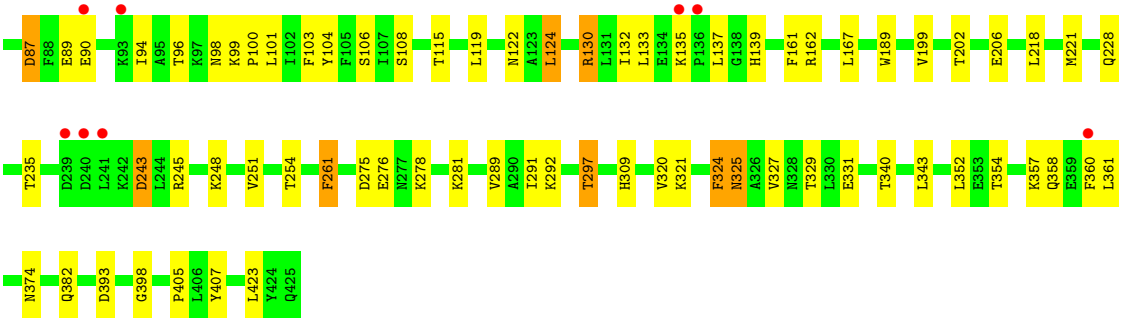


• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain C:

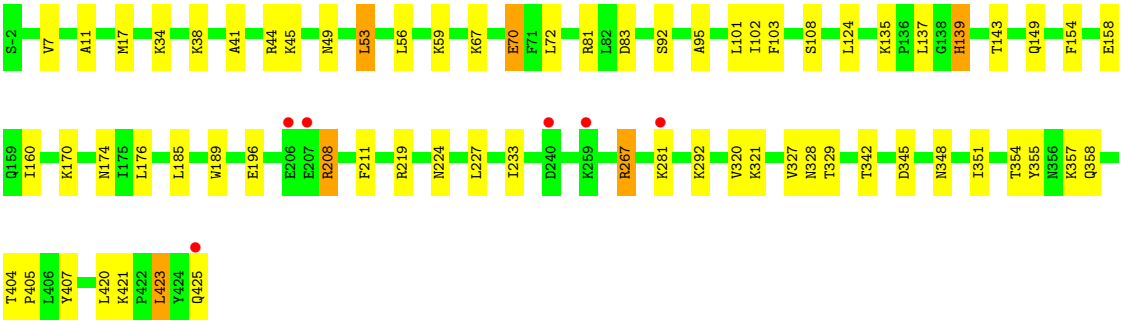






• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.87Å 153.87Å 250.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.08 – 2.75 52.08 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.08-2.75) 100.0 (52.08-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.254 0.218 , 0.251	Depositor DCC
R_{free} test set	1994 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14155	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0.44	0/3602	0.63	0/4862
1	B	0.45	0/3602	0.60	0/4862
1	C	0.48	1/3602 (0.0%)	0.65	0/4862
1	D	0.53	0/3602	0.63	0/4862
All	All	0.48	1/14408 (0.0%)	0.63	0/19448

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	357	LYS	C-N	-5.51	1.21	1.34

There are no bond angle outliers.

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	3522	0	3533	31	0
1	B	3522	0	3533	58	0
1	C	3522	0	3533	53	0
1	D	3522	0	3533	31	0
2	A	14	0	0	3	0
2	B	18	0	0	0	0
2	C	17	0	0	3	0
2	D	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14155	0	14132	170	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 (170) 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:B:60:THR:HG21	1:B:62:LEU:HD22	1.38	1.04
1:D:92:SER:HB3	1:D:124:LEU:HD11	1.47	0.95
1:C:1:MET:O	1:C:34:LYS:HG2	1.70	0.91
1:B:45:LYS:H	1:B:45:LYS:HE2	1.33	0.90
1:D:17:MET:HE1	1:D:56:LEU:HA	1.59	0.82
1:B:45:LYS:H	1:B:45:LYS:CE	1.92	0.81
1:D:67:LYS:HE2	1:D:70:GLU:HG3	1.62	0.79
1:B:60:THR:HG22	1:B:62:LEU:H	1.48	0.78
1:D:267:ARG:NH1	1:D:404:THR:O	2.21	0.73
1:D:170:LYS:NZ	1:D:174:ASN:OD1	2.21	0.73
1:B:133:LEU:O	1:B:163:ILE:HG22	1.90	0.72
1:B:44:ARG:HD3	1:B:82:LEU:HG	1.73	0.70
1:B:62:LEU:HD12	1:B:65:ARG:HD3	1.71	0.70
1:C:100:PRO:HB3	1:C:130:ARG:HH21	1.57	0.69
1:B:45:LYS:HE2	1:B:45:LYS:N	2.08	0.69
1:B:96:THR:HG21	1:B:99:LYS:HE2	1.75	0.69
1:B:25:TYR:OH	1:B:66:GLU:HG2	1.95	0.67
1:B:44:ARG:NH1	1:B:82:LEU:HD23	2.10	0.67
1:C:130:ARG:NH1	1:C:374:ASN:OD1	2.31	0.64
1:D:92:SER:HB2	1:D:124:LEU:HD21	1.80	0.63
1:A:375:ASN:ND2	2:A:502:HOH:O	2.32	0.62
1:D:92:SER:CB	1:D:124:LEU:HD21	2.30	0.62
1:B:327:VAL:HG21	1:B:344:LYS:HD2	1.82	0.61
1:A:355:TYR:CZ	1:A:357:LYS:HG2	2.36	0.60
1:B:60:THR:HG22	1:B:62:LEU:N	2.17	0.60
1:D:355:TYR:CE2	1:D:357:LYS:HD3	2.37	0.59
1:C:96:THR:HG21	1:C:99:LYS:HE2	1.84	0.58
1:C:130:ARG:HH12	1:C:374:ASN:HB2	1.66	0.58
1:B:10:GLY:HA3	1:B:106:SER:O	2.04	0.58
1:A:105:PHE:CZ	1:A:131:LEU:HD11	2.38	0.57
1:D:92:SER:HA	1:D:95:ALA:CB	2.35	0.57
1:B:60:THR:HG21	1:B:62:LEU:CD2	2.26	0.56
1:D:11:ALA:CB	1:D:41:ALA:HB1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:LYS:HE2	1:D:425:GLN:NE2	2.21	0.56
1:B:45:LYS:N	1:B:45:LYS:CD	2.69	0.55
1:A:183:PRO:O	1:A:187:ILE:HD12	2.07	0.54
1:C:12:THR:OG1	1:C:44:ARG:NH2	2.40	0.54
1:B:84:ASN:C	1:B:84:ASN:HD22	2.11	0.53
1:C:14:ASP:O	1:C:18:ARG:HG3	2.08	0.53
1:B:29:THR:HG22	1:B:67:LYS:HE3	1.89	0.53
1:A:6:LEU:HD12	1:A:102:ILE:HB	1.89	0.53
1:C:78:PHE:HZ	1:C:90:GLU:HG3	1.73	0.53
1:B:60:THR:CG2	1:B:62:LEU:HB2	2.39	0.52
1:C:49:ASN:O	1:C:53:LEU:HD23	2.09	0.52
1:A:47:LEU:HD12	1:A:77:TYR:CE2	2.45	0.52
1:B:82:LEU:HD12	1:B:82:LEU:N	2.25	0.52
1:C:243:ASP:OD1	1:C:243:ASP:C	2.48	0.52
1:C:130:ARG:HG3	1:C:161:PHE:HE1	1.76	0.51
1:D:233:ILE:HD11	1:D:320:VAL:HG11	1.92	0.51
1:C:321:LYS:NZ	2:C:504:HOH:O	2.43	0.51
1:A:281:LYS:HD3	1:A:281:LYS:H	1.75	0.51
1:B:45:LYS:H	1:B:45:LYS:CD	2.22	0.51
1:C:30:HIS:HE1	1:C:360:PHE:HD2	1.59	0.51
1:C:44:ARG:CZ	1:C:44:ARG:H	2.23	0.51
1:B:210:GLU:HB3	1:B:278:LYS:HE3	1.92	0.50
1:B:44:ARG:HH11	1:B:82:LEU:HD23	1.74	0.50
1:B:66:GLU:H	1:B:66:GLU:CD	2.13	0.50
1:D:328:ASN:HA	1:D:342:THR:O	2.12	0.50
1:B:45:LYS:CE	1:B:45:LYS:N	2.71	0.50
1:C:393:ASP:OD1	2:C:501:HOH:O	2.20	0.50
1:C:30:HIS:HE1	1:C:360:PHE:CD2	2.29	0.49
1:B:45:LYS:N	1:B:45:LYS:HD3	2.28	0.49
1:A:281:LYS:HE2	1:B:45:LYS:NZ	2.28	0.49
1:B:114:THR:CG2	1:B:115:THR:N	2.75	0.49
1:B:210:GLU:HB3	1:B:278:LYS:CE	2.43	0.48
1:C:124:LEU:HD12	1:C:124:LEU:HA	1.67	0.48
1:C:7:VAL:HG11	1:C:103:PHE:CE1	2.49	0.48
1:B:405:PRO:HG2	1:B:407:TYR:CZ	2.49	0.48
1:C:89:GLU:HG3	1:C:122:ASN:OD1	2.14	0.48
1:D:38:LYS:NZ	2:D:504:HOH:O	2.47	0.47
1:A:167:LEU:HD21	1:A:228:GLN:HG2	1.96	0.47
1:D:49:ASN:O	1:D:53:LEU:HD22	2.13	0.47
1:A:103:PHE:HB2	1:A:131:LEU:HD12	1.97	0.47
1:D:281:LYS:O	1:D:281:LYS:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:SER:O	1:B:421:LYS:HG3	2.15	0.47
1:C:325:ASN:N	2:C:507:HOH:O	2.46	0.47
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.78	0.47
1:C:104:TYR:CE2	1:C:132:ILE:HG21	2.49	0.47
1:D:405:PRO:HG2	1:D:407:TYR:CZ	2.49	0.47
1:B:60:THR:CG2	1:B:62:LEU:HD22	2.27	0.47
1:C:5:ASP:OD1	1:C:38:LYS:HB2	2.14	0.47
1:B:49:ASN:O	1:B:53:LEU:HD23	2.14	0.47
1:B:82:LEU:HD12	1:B:82:LEU:H	1.79	0.47
1:B:114:THR:HG22	1:B:115:THR:N	2.30	0.47
1:C:25:TYR:CE1	1:C:29:THR:HG21	2.49	0.47
1:C:167:LEU:HD21	1:C:228:GLN:HG2	1.96	0.47
1:B:170:LYS:NZ	1:B:174:ASN:OD1	2.47	0.47
1:C:324:PHE:O	1:C:325:ASN:ND2	2.48	0.47
1:B:281:LYS:HD3	1:B:281:LYS:H	1.80	0.47
1:D:345:ASP:OD1	1:D:348:ASN:N	2.41	0.47
1:B:82:LEU:H	1:B:82:LEU:CD1	2.28	0.46
1:D:44:ARG:HG2	1:D:81:ARG:HA	1.97	0.46
1:C:261:PHE:CZ	1:C:398:GLY:HA3	2.50	0.46
1:B:2:LEU:H	1:B:2:LEU:HG	1.49	0.46
1:D:92:SER:HA	1:D:95:ALA:HB3	1.95	0.46
1:A:164:ASP:OD1	1:A:225:HIS:ND1	2.43	0.46
1:A:352:LEU:N	1:A:352:LEU:HD23	2.29	0.46
1:B:135:LYS:HE2	1:B:135:LYS:HB2	1.72	0.46
1:A:261:PHE:CZ	1:A:398:GLY:HA3	2.51	0.45
1:D:7:VAL:HB	1:D:103:PHE:CD1	2.51	0.45
1:A:169:LYS:NZ	2:A:504:HOH:O	2.50	0.45
1:A:95:ALA:HB1	1:A:101:LEU:HD22	1.98	0.45
1:C:325:ASN:O	1:C:327:VAL:N	2.50	0.45
1:B:245:ARG:CG	1:B:245:ARG:HH11	2.30	0.45
1:C:221:MET:HG3	1:C:309:HIS:NE2	2.32	0.45
1:D:208:ARG:O	1:D:208:ARG:HG3	2.17	0.45
1:D:139:HIS:CE1	1:D:143:THR:HG21	2.52	0.45
1:C:361:LEU:HD23	1:C:361:LEU:HA	1.77	0.44
1:B:60:THR:HG23	1:B:62:LEU:HD13	1.99	0.44
1:A:199:VAL:O	1:A:309:HIS:HA	2.18	0.44
1:C:1:MET:O	1:C:34:LYS:CG	2.54	0.44
1:C:81:ARG:NH2	1:C:87:ASP:OD1	2.50	0.44
1:A:112:PHE:HB3	1:A:151:ILE:HD11	1.99	0.44
1:B:24:LEU:HD13	1:B:39:ILE:HD13	2.00	0.44
1:B:91:LEU:HD13	1:B:124:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.85	0.44
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.84	0.44
1:C:82:LEU:HD22	1:C:115:THR:OG1	2.18	0.44
1:C:248:LYS:O	1:C:251:VAL:HG12	2.18	0.44
1:A:405:PRO:HG2	1:A:407:TYR:CZ	2.53	0.44
1:B:56:LEU:O	1:B:60:THR:HB	2.17	0.44
1:A:375:ASN:CG	2:A:502:HOH:O	2.55	0.43
1:C:14:ASP:OD2	1:C:18:ARG:HD2	2.17	0.43
1:C:24:LEU:HG	1:C:39:ILE:HD13	2.00	0.43
1:D:355:TYR:HE2	1:D:357:LYS:HD3	1.84	0.43
1:A:3:ASP:HB2	1:A:34:LYS:HD3	1.99	0.43
1:C:254:THR:HG21	1:C:297:THR:HG23	2.00	0.43
1:C:343:LEU:HD12	1:C:352:LEU:HD21	1.99	0.43
1:C:44:ARG:HG2	1:C:45:LYS:N	2.32	0.43
1:C:100:PRO:HB3	1:C:130:ARG:NH2	2.27	0.43
1:D:70:GLU:H	1:D:70:GLU:HG2	1.04	0.43
1:A:77:TYR:HD1	1:A:78:PHE:N	2.17	0.43
1:A:53:LEU:HD12	1:A:72:LEU:HD22	2.01	0.43
1:C:325:ASN:HD22	1:C:325:ASN:C	2.22	0.43
1:A:53:LEU:HA	1:A:53:LEU:HD13	1.65	0.43
1:A:328:ASN:HA	1:A:342:THR:O	2.19	0.43
1:C:16:ALA:HA	1:C:20:LEU:HB2	2.01	0.42
1:D:196:GLU:HB2	1:D:321:LYS:HB2	2.02	0.42
1:A:281:LYS:HE2	1:B:45:LYS:HD2	2.01	0.42
1:C:130:ARG:CG	1:C:161:PHE:HE1	2.33	0.42
1:C:34:LYS:HB3	1:C:34:LYS:NZ	2.34	0.42
1:D:17:MET:HE2	1:D:59:LYS:HB2	2.02	0.42
1:B:198:CYS:O	1:B:318:ALA:HA	2.18	0.42
1:C:405:PRO:HG2	1:C:407:TYR:CZ	2.54	0.42
1:D:292:LYS:CE	1:D:423:LEU:O	2.67	0.42
1:B:164:ASP:OD1	1:B:225:HIS:ND1	2.46	0.42
1:B:245:ARG:CZ	1:B:381:HIS:HB2	2.49	0.42
1:A:281:LYS:CE	1:B:45:LYS:NZ	2.83	0.41
1:A:16:ALA:HA	1:A:20:LEU:HB2	2.02	0.41
1:A:88:PHE:CG	1:A:118:ASN:HB3	2.55	0.41
1:B:210:GLU:H	1:B:210:GLU:HG2	1.47	0.41
1:C:162:ARG:CZ	1:C:382:GLN:HG2	2.50	0.41
1:C:275:ASP:O	1:C:275:ASP:OD1	2.38	0.41
1:B:84:ASN:HD22	1:B:85:PRO:N	2.18	0.41
1:C:9:PHE:O	1:C:106:SER:HB3	2.20	0.41
1:D:11:ALA:HB1	1:D:41:ALA:HB1	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HG12	1:A:130:ARG:HB2	2.03	0.41
1:C:199:VAL:O	1:C:309:HIS:HA	2.20	0.41
1:C:320:VAL:O	1:C:331:GLU:HA	2.20	0.41
1:C:53:LEU:HD13	1:C:53:LEU:HA	1.95	0.41
1:C:292:LYS:CE	1:C:423:LEU:O	2.68	0.41
1:A:25:TYR:OH	1:A:66:GLU:HG2	2.21	0.41
1:B:261:PHE:CZ	1:B:398:GLY:HA3	2.55	0.40
1:C:83:ASP:OD1	1:C:84:ASN:N	2.54	0.40
1:C:218:LEU:HD13	1:C:291:ILE:HD11	2.03	0.40
1:B:327:VAL:O	1:B:342:THR:HG22	2.21	0.40
1:D:92:SER:HA	1:D:95:ALA:HB2	2.04	0.40
1:D:420:LEU:HD22	1:D:423:LEU:HD12	2.03	0.40
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.76	0.40
1:B:135:LYS:H	1:B:135:LYS:HG3	1.44	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	426/428 (100%)	411 (96%)	15 (4%)	0	100	100
1	B	426/428 (100%)	422 (99%)	4 (1%)	0	100	100
1	C	426/428 (100%)	416 (98%)	10 (2%)	0	100	100
1	D	426/428 (100%)	414 (97%)	12 (3%)	0	100	100
All	All	1704/1712 (100%)	1663 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	389/389 (100%)	358 (92%)	31 (8%)	12 21
1	B	389/389 (100%)	343 (88%)	46 (12%)	5 8
1	C	389/389 (100%)	347 (89%)	42 (11%)	6 10
1	D	389/389 (100%)	358 (92%)	31 (8%)	12 21
All	All	1556/1556 (100%)	1406 (90%)	150 (10%)	8 14

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	45	LYS
1	A	53	LEU
1	A	63	HIS
1	A	66	GLU
1	A	77	TYR
1	A	84	ASN
1	A	108	SER
1	A	117	GLN
1	A	158	GLU
1	A	163	ILE
1	A	189	TRP
1	A	221	MET
1	A	224	ASN
1	A	241	LEU
1	A	261	PHE
1	A	281	LYS
1	A	289	VAL
1	A	325	ASN
1	A	329	THR
1	A	340	THR
1	A	354	THR
1	A	357	LYS
1	A	358	GLN

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Mol	Chain	Res	Type
1	A	359	GLU
1	A	361	LEU
1	A	362	GLN
1	A	375	ASN
1	A	388	SER
1	A	411	SER
1	A	425	GLN
1	B	-2	SER
1	B	2	LEU
1	B	45	LYS
1	B	46	GLU
1	B	59	LYS
1	B	60	THR
1	B	62	LEU
1	B	66	GLU
1	B	82	LEU
1	B	84	ASN
1	B	91	LEU
1	B	113	THR
1	B	114	THR
1	B	119	LEU
1	B	124	LEU
1	B	135	LYS
1	B	137	LEU
1	B	152	SER
1	B	176	LEU
1	B	189	TRP
1	B	207	GLU
1	B	208	ARG
1	B	210	GLU
1	B	235	THR
1	B	236	ASP
1	B	241	LEU
1	B	245	ARG
1	B	251	VAL
1	B	267	ARG
1	B	281	LYS
1	B	289	VAL
1	B	297	THR
1	B	322	ILE
1	B	325	ASN
1	B	327	VAL

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Mol	Chain	Res	Type
1	B	329	THR
1	B	336	GLN
1	B	340	THR
1	B	343	LEU
1	B	345	ASP
1	B	346	HIS
1	B	354	THR
1	B	357	LYS
1	B	358	GLN
1	B	396	ILE
1	B	418	GLU
1	C	-2	SER
1	C	7	VAL
1	C	24	LEU
1	C	34	LYS
1	C	35	LYS
1	C	44	ARG
1	C	50	GLU
1	C	56	LEU
1	C	62	LEU
1	C	63	HIS
1	C	70	GLU
1	C	76	SER
1	C	87	ASP
1	C	94	ILE
1	C	98	ASN
1	C	101	LEU
1	C	108	SER
1	C	119	LEU
1	C	124	LEU
1	C	130	ARG
1	C	133	LEU
1	C	135	LYS
1	C	137	LEU
1	C	139	HIS
1	C	189	TRP
1	C	202	THR
1	C	206	GLU
1	C	235	THR
1	C	243	ASP
1	C	245	ARG
1	C	261	PHE

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Mol	Chain	Res	Type
1	C	276	GLU
1	C	278	LYS
1	C	281	LYS
1	C	289	VAL
1	C	297	THR
1	C	324	PHE
1	C	325	ASN
1	C	329	THR
1	C	340	THR
1	C	354	THR
1	C	358	GLN
1	D	34	LYS
1	D	45	LYS
1	D	53	LEU
1	D	70	GLU
1	D	72	LEU
1	D	83	ASP
1	D	101	LEU
1	D	102	ILE
1	D	108	SER
1	D	135	LYS
1	D	137	LEU
1	D	139	HIS
1	D	149	GLN
1	D	154	PHE
1	D	158	GLU
1	D	160	ILE
1	D	176	LEU
1	D	185	LEU
1	D	189	TRP
1	D	208	ARG
1	D	211	PHE
1	D	219	ARG
1	D	224	ASN
1	D	227	LEU
1	D	267	ARG
1	D	327	VAL
1	D	329	THR
1	D	351	ILE
1	D	354	THR
1	D	358	GLN
1	D	423	LEU

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

Mol	Chain	Res	Type
1	A	336	GLN
1	B	84	ASN
1	B	122	ASN
1	B	325	ASN
1	B	328	ASN
1	B	412	HIS
1	C	30	HIS
1	C	325	ASN
1	D	412	HIS
1	D	425	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	428/428 (100%)	0.21	23 (5%)	25	31	30, 62, 107, 135	0
1	B	428/428 (100%)	-0.03	7 (1%)	72	79	28, 45, 82, 120	0
1	C	428/428 (100%)	0.09	15 (3%)	44	52	32, 54, 96, 122	0
1	D	428/428 (100%)	0.02	6 (1%)	75	82	24, 50, 84, 113	0
All	All	1712/1712 (100%)	0.07	51 (2%)	50	59	24, 51, 97, 135	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	GLU	4.7
1	A	346	HIS	4.4
1	A	53	LEU	4.3
1	B	425	GLN	4.2
1	A	135	LYS	4.2
1	A	57	CYS	4.1
1	A	63	HIS	3.9
1	B	206	GLU	3.9
1	C	241	LEU	3.8
1	A	55	LEU	3.3
1	C	36	ASP	3.2
1	C	135	LYS	3.2
1	D	259	LYS	3.2
1	A	52	PHE	3.1
1	C	57	CYS	3.1
1	A	425	GLN	3.1
1	C	90	GLU	3.1
1	C	360	PHE	3.0
1	D	425	GLN	2.9
1	B	235	THR	2.9
1	C	50	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLU	2.9
1	A	360	PHE	2.8
1	A	59	LYS	2.8
1	B	-2	SER	2.8
1	A	56	LEU	2.7
1	C	136	PRO	2.7
1	A	69	GLU	2.6
1	D	207	GLU	2.5
1	C	93	LYS	2.4
1	A	98	ASN	2.4
1	C	78	PHE	2.4
1	B	135	LYS	2.4
1	B	207	GLU	2.4
1	A	62	LEU	2.3
1	D	240	ASP	2.3
1	A	60	THR	2.3
1	A	78	PHE	2.3
1	A	70	GLU	2.3
1	D	206	GLU	2.3
1	C	-2	SER	2.2
1	C	58	GLU	2.2
1	C	239	ASP	2.1
1	B	259	LYS	2.1
1	D	281	LYS	2.1
1	A	51	GLU	2.1
1	A	47	LEU	2.1
1	A	93	LYS	2.1
1	C	240	ASP	2.0
1	C	47	LEU	2.0
1	A	-2	SER	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.