



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 PM UTC

PDB ID : 8I37 / pdb_00008i37
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

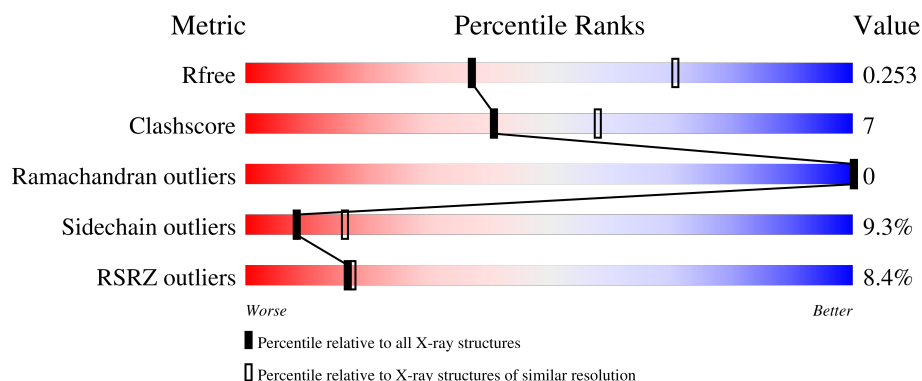
1 Overall quality at a glance

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	11% 82% 16% .
1	B	428	8% 80% 16% .
1	C	428	10% 73% 22% .
1	D	428	5% 83% 15% .

2 Entry composition

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

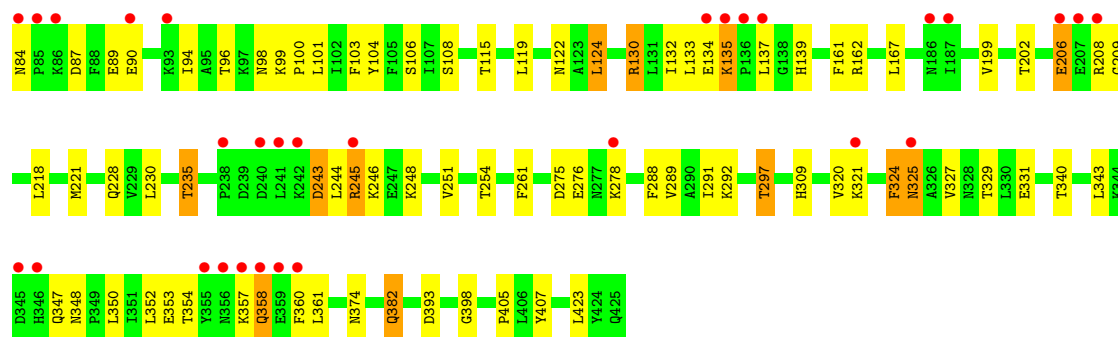
- Molecule 2 is water.

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

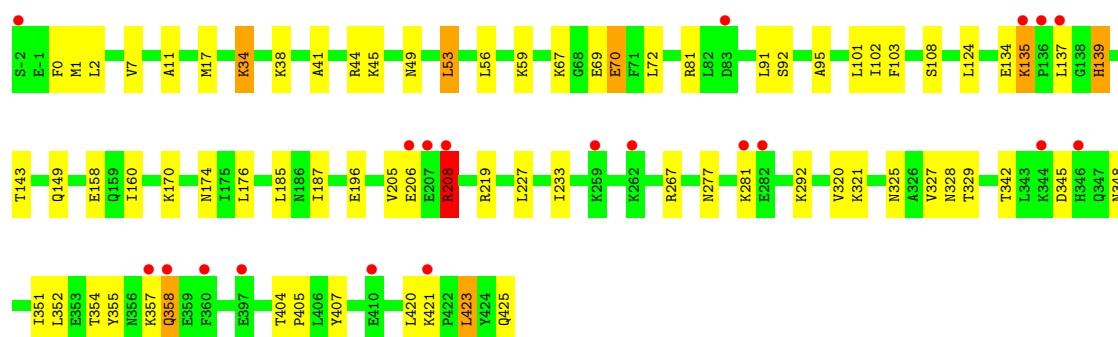
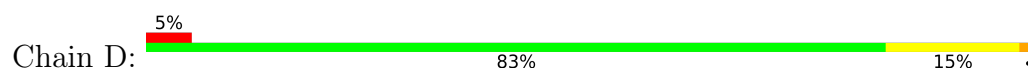
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	17	Total	O	0	0
			17	17		
2	D	18	Total	O	0	0
			18	18		



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



4 Data and refinement statistics

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) 99.9 (52.08-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.254 0.221 , 0.253	Depositor DCC
R_{free} test set	1994 reflections (2.22%)	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)	0.35 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.56	1/3602 (0.0%)	0.68	7/4862 (0.1%)
1	B	0.56	3/3602 (0.1%)	0.66	8/4862 (0.2%)
1	C	0.62	1/3602 (0.0%)	0.75	13/4862 (0.3%)
1	D	0.72	1/3602 (0.0%)	0.74	12/4862 (0.2%)
All	All	0.62	6/14408 (0.0%)	0.71	40/19448 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	357	LYS	C-N	-9.21	1.21	1.33
1	A	325	ASN	C-O	-6.62	1.19	1.24
1	D	0	PHE	CA-C	-5.58	1.46	1.52
1	B	137	LEU	CA-C	-5.23	1.47	1.53
1	B	355	TYR	CA-C	-5.23	1.46	1.52
1	B	325	ASN	CA-C	-5.22	1.46	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	GLU	N-CA-C	9.11	122.41	111.02
1	A	206	GLU	N-CA-C	8.90	122.14	111.02
1	D	1	MET	N-CA-C	8.85	123.68	111.74
1	C	206	GLU	N-CA-C	8.65	121.03	110.91
1	D	358	GLN	N-CA-C	8.61	121.43	110.24
1	B	-1	GLU	N-CA-C	-8.43	101.33	111.69
1	C	208	ARG	N-CA-C	-8.31	103.30	113.19
1	C	358	GLN	N-CA-C	7.94	121.70	110.50
1	D	2	LEU	N-CA-C	7.46	121.05	110.23
1	C	347	GLN	N-CA-C	7.20	122.26	112.68
1	C	353	GLU	N-CA-C	7.19	120.38	109.23
1	A	361	LEU	N-CA-C	-7.01	97.87	108.52
1	D	208	ARG	N-CA-C	-6.90	102.91	112.30
1	B	353	GLU	N-CA-C	6.81	120.27	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	GLN	N-CA-C	-6.80	97.54	108.55
1	C	135	LYS	N-CA-C	6.59	121.71	112.75
1	A	97	LYS	N-CA-C	6.48	121.18	113.28
1	C	2	LEU	N-CA-C	6.38	119.49	110.23
1	A	325	ASN	N-CA-C	-6.22	99.65	108.23
1	C	134	GLU	N-CA-C	6.02	117.81	110.41
1	C	235	THR	CB-CA-C	-6.01	99.37	109.65
1	D	134	GLU	N-CA-C	5.91	118.17	110.43
1	C	209	GLY	N-CA-C	5.83	121.45	113.99
1	B	329	THR	N-CA-C	5.74	118.47	108.76
1	D	205	VAL	CB-CA-C	5.54	119.28	112.02
1	B	4	PHE	N-CA-C	5.46	117.39	108.76
1	B	325	ASN	N-CA-C	-5.40	101.11	108.24
1	D	135	LYS	N-CA-C	5.40	120.96	113.45
1	B	324	PHE	N-CA-C	-5.38	106.84	113.41
1	D	34	LYS	N-CA-C	-5.34	102.58	110.48
1	D	325	ASN	N-CA-C	-5.29	99.53	110.80
1	A	0	PHE	N-CA-C	5.28	122.05	110.80
1	B	236	ASP	N-CA-C	-5.25	101.88	109.59
1	A	60	THR	N-CA-C	5.21	120.49	113.72
1	C	348	ASN	CA-C-N	-5.20	114.63	120.14
1	C	348	ASN	C-N-CA	-5.20	114.63	120.14
1	C	1	MET	N-CA-C	5.18	118.73	111.74
1	A	362	GLN	CB-CA-C	5.06	117.42	109.27
1	D	135	LYS	CA-C-N	-5.06	114.22	120.79
1	D	135	LYS	C-N-CA	-5.06	114.22	120.79

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	36	0
1	B	3522	0	3533	62	0
1	C	3522	0	3533	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3522	0	3533	34	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
All	All	14155	0	14132	184	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 7.

All (184) 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:B:45:LYS:H	1:B:45:LYS:CE	1.92	0.81
1:D:17:MET:HE1	1:D:56:LEU:HA	1.63	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ASN:C	1:B:84:ASN:HD22	2.11	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:D:17:MET:HE2	1:D:59:LYS:HB2	1.86	0.57
1:B:60:THR:HG21	1:B:62:LEU:CD2	2.26	0.56
1:C:243:ASP:OD1	1:C:243:ASP:C	2.48	0.56
1:D:11:ALA:CB	1:D:41:ALA:HB1	2.35	0.56
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:B:66:GLU:H	1:B:66:GLU:CD	2.13	0.54
1:C:12:THR:OG1	1:C:44:ARG:NH2	2.40	0.54
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: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: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:A:281:LYS:CE	1:B:45:LYS:HZ2	2.24	0.50
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: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:321:LYS:NZ	2:C:504:HOH:O	2.43	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:325:ASN:HD22	1:C:325:ASN:C	2.22	0.48
1:D:91:LEU:O	1:D:92:SER:OG	2.28	0.48
1:A:375:ASN:CG	2:A:502:HOH:O	2.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:288:PHE:C	1:B:288:PHE:CD1	2.95	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:A:84:ASN:C	1:A:84:ASN:HD22	2.26	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
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: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:A:288:PHE:CD1	1:A:288:PHE:C	2.96	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: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:244:LEU:O	1:C:245:ARG:C	2.61	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:B:198:CYS:O	1:B:318:ALA:HA	2.18	0.42
1:C:288:PHE:C	1:C:288:PHE:CD1	2.97	0.42
1:C:405:PRO:HG2	1:C:407:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:313:MET:HE1	1:A:414:LEU:HD23	2.02	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
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:230:LEU:C	1:C:230:LEU:HD23	2.46	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:281:LYS:CE	1:B:45:LYS:NZ	2.83	0.41
1:A:281:LYS:HE2	1:B:45:LYS:HZ2	1.85	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:C:245:ARG:O	1:C:246:LYS:C	2.64	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:D:17:MET:HE1	1:D:56:LEU:HD12	2.02	0.40
1:B:135:LYS:H	1:B:135:LYS:HG3	1.44	0.40
1:B:245:ARG:O	1:B:246:LYS:C	2.63	0.40
1:C:275:ASP:HB2	1:D:277:ASN:CG	2.46	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	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

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%)	357 (92%)	32 (8%)	10	20
1	B	389/389 (100%)	346 (89%)	43 (11%)	6	11
1	C	389/389 (100%)	348 (90%)	41 (10%)	6	13
1	D	389/389 (100%)	361 (93%)	28 (7%)	13	25
All	All	1556/1556 (100%)	1412 (91%)	144 (9%)	8	16

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	44	ARG

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Mol	Chain	Res	Type
1	A	45	LYS
1	A	53	LEU
1	A	63	HIS
1	A	66	GLU
1	A	97	LYS
1	A	108	SER
1	A	117	GLN
1	A	135	LYS
1	A	158	GLU
1	A	163	ILE
1	A	221	MET
1	A	241	LEU
1	A	281	LYS
1	A	289	VAL
1	A	325	ASN
1	A	327	VAL
1	A	329	THR
1	A	340	THR
1	A	350	LEU
1	A	352	LEU
1	A	354	THR
1	A	357	LYS
1	A	358	GLN
1	A	359	GLU
1	A	361	LEU
1	A	375	ASN
1	A	388	SER
1	A	411	SER
1	A	418	GLU
1	A	425	GLN
1	B	-2	SER
1	B	2	LEU
1	B	45	LYS
1	B	46	GLU
1	B	60	THR
1	B	62	LEU
1	B	66	GLU
1	B	82	LEU
1	B	86	LYS
1	B	91	LEU
1	B	113	THR
1	B	114	THR

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Mol	Chain	Res	Type
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	207	GLU
1	B	208	ARG
1	B	210	GLU
1	B	221	MET
1	B	235	THR
1	B	241	LEU
1	B	245	ARG
1	B	251	VAL
1	B	267	ARG
1	B	289	VAL
1	B	297	THR
1	B	322	ILE
1	B	325	ASN
1	B	327	VAL
1	B	329	THR
1	B	336	GLN
1	B	340	THR
1	B	343	LEU
1	B	345	ASP
1	B	350	LEU
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	2	LEU
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

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Mol	Chain	Res	Type
1	C	70	GLU
1	C	76	SER
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	202	THR
1	C	206	GLU
1	C	235	THR
1	C	243	ASP
1	C	245	ARG
1	C	276	GLU
1	C	278	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	350	LEU
1	C	354	THR
1	C	358	GLN
1	C	382	GLN
1	D	34	LYS
1	D	45	LYS
1	D	53	LEU
1	D	69	GLU
1	D	70	GLU
1	D	72	LEU
1	D	101	LEU
1	D	102	ILE
1	D	108	SER
1	D	135	LYS
1	D	137	LEU
1	D	139	HIS

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Mol	Chain	Res	Type
1	D	149	GLN
1	D	158	GLU
1	D	160	ILE
1	D	176	LEU
1	D	185	LEU
1	D	187	ILE
1	D	208	ARG
1	D	219	ARG
1	D	227	LEU
1	D	327	VAL
1	D	329	THR
1	D	351	ILE
1	D	352	LEU
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	323	HIS
1	A	328	ASN
1	A	336	GLN
1	B	84	ASN
1	B	165	HIS
1	B	269	GLN
1	B	325	ASN
1	B	328	ASN
1	B	336	GLN
1	B	412	HIS
1	C	30	HIS
1	C	165	HIS
1	C	325	ASN
1	C	336	GLN
1	C	375	ASN
1	C	381	HIS
1	C	382	GLN
1	D	126	HIS
1	D	139	HIS
1	D	165	HIS
1	D	336	GLN

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Mol	Chain	Res	Type
1	D	375	ASN
1	D	425	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	428/428 (100%)	0.76	49 (11%) 10 8	30, 62, 107, 135	0
1	B	428/428 (100%)	0.24	33 (7%) 19 19	28, 45, 82, 120	0
1	C	428/428 (100%)	0.60	42 (9%) 13 12	32, 54, 96, 122	0
1	D	428/428 (100%)	0.35	20 (4%) 36 36	24, 50, 84, 113	0
All	All	1712/1712 (100%)	0.49	144 (8%) 17 17	24, 51, 97, 135	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	PHE	6.7
1	B	206	GLU	6.5
1	C	360	PHE	6.3
1	B	135	LYS	6.1
1	C	136	PRO	5.9
1	D	281	LYS	5.9
1	C	135	LYS	5.6
1	B	207	GLU	5.6
1	A	96	THR	5.3
1	B	235	THR	5.1
1	B	236	ASP	5.0
1	C	241	LEU	5.0
1	C	84	ASN	4.9
1	D	207	GLU	4.8
1	A	135	LYS	4.5
1	A	355	TYR	4.4
1	B	82	LEU	4.3
1	A	136	PRO	4.2
1	D	206	GLU	4.1
1	A	356	ASN	4.1
1	D	136	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	347	GLN	4.0
1	D	358	GLN	4.0
1	C	134	GLU	3.9
1	A	35	LYS	3.9
1	B	-2	SER	3.9
1	C	90	GLU	3.8
1	A	63	HIS	3.8
1	D	208	ARG	3.8
1	A	121	GLN	3.7
1	A	418	GLU	3.7
1	C	137	LEU	3.7
1	B	277	ASN	3.7
1	D	135	LYS	3.7
1	C	346	HIS	3.6
1	A	278	LYS	3.6
1	C	357	LYS	3.5
1	C	93	LYS	3.4
1	A	357	LYS	3.4
1	A	45	LYS	3.4
1	C	238	PRO	3.4
1	A	110	SER	3.3
1	B	134	GLU	3.3
1	C	206	GLU	3.3
1	B	355	TYR	3.3
1	C	63	HIS	3.3
1	B	136	PRO	3.2
1	C	82	LEU	3.2
1	B	358	GLN	3.2
1	C	356	ASN	3.2
1	C	-2	SER	3.2
1	A	94	ILE	3.2
1	C	187	ILE	3.2
1	A	86	LYS	3.1
1	A	-2	SER	3.1
1	C	44	ARG	3.1
1	B	211	PHE	3.0
1	C	3	ASP	3.0
1	A	0	PHE	3.0
1	A	361	LEU	2.9
1	C	85	PRO	2.9
1	C	359	GLU	2.9
1	A	58	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	44	ARG	2.8
1	A	57	CYS	2.8
1	A	346	HIS	2.8
1	C	240	ASP	2.8
1	A	206	GLU	2.8
1	D	360	PHE	2.8
1	A	93	LYS	2.8
1	A	211	PHE	2.8
1	A	18	ARG	2.8
1	C	358	GLN	2.7
1	A	69	GLU	2.7
1	B	205	VAL	2.7
1	B	345	ASP	2.7
1	C	345	ASP	2.7
1	C	325	ASN	2.7
1	B	360	PHE	2.7
1	A	83	ASP	2.7
1	B	425	GLN	2.6
1	A	208	ARG	2.6
1	C	45	LYS	2.6
1	A	358	GLN	2.6
1	A	66	GLU	2.6
1	A	112	PHE	2.6
1	C	81	ARG	2.6
1	C	207	GLU	2.6
1	C	186	ASN	2.6
1	D	-2	SER	2.5
1	B	208	ARG	2.5
1	C	208	ARG	2.5
1	A	240	ASP	2.5
1	A	281	LYS	2.5
1	A	158	GLU	2.5
1	B	381	HIS	2.5
1	D	346	HIS	2.5
1	B	242	LYS	2.4
1	C	242	LYS	2.4
1	B	210	GLU	2.4
1	D	397	GLU	2.4
1	C	321	LYS	2.4
1	A	154	PHE	2.4
1	A	126	HIS	2.4
1	B	157	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	86	LYS	2.4
1	A	113	THR	2.4
1	B	278	LYS	2.4
1	B	281	LYS	2.3
1	C	278	LYS	2.3
1	A	348	ASN	2.3
1	D	282	GLU	2.3
1	D	83	ASP	2.3
1	A	98	ASN	2.3
1	B	349	PRO	2.3
1	B	357	LYS	2.3
1	D	344	LYS	2.3
1	A	421	LYS	2.2
1	B	282	GLU	2.2
1	A	82	LEU	2.2
1	A	187	ILE	2.2
1	B	259	LYS	2.2
1	D	259	LYS	2.2
1	A	209	GLY	2.2
1	A	3	ASP	2.2
1	C	35	LYS	2.2
1	D	421	LYS	2.2
1	C	57	CYS	2.2
1	B	348	ASN	2.2
1	D	357	LYS	2.2
1	C	36	ASP	2.2
1	A	109	PRO	2.1
1	D	137	LEU	2.1
1	C	67	LYS	2.1
1	C	355	TYR	2.1
1	B	138	GLY	2.1
1	A	78	PHE	2.1
1	B	3	ASP	2.0
1	C	83	ASP	2.0
1	D	410	GLU	2.0
1	D	262	LYS	2.0
1	C	245	ARG	2.0
1	A	207	GLU	2.0
1	B	19	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 oligosaccharides 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.