Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 10:37 PM EDT

PDB ID	:	1XGV
Title	:	Isocitrate Dehydrogenase from the hyperthermophile Aeropyrum pernix
Authors	:	Karlstrom, M.; Stokke, R.; Steen, I.H.; Birkeland, N.-K.; Ladenstein, R.
Deposited on	:	2004-09-17
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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
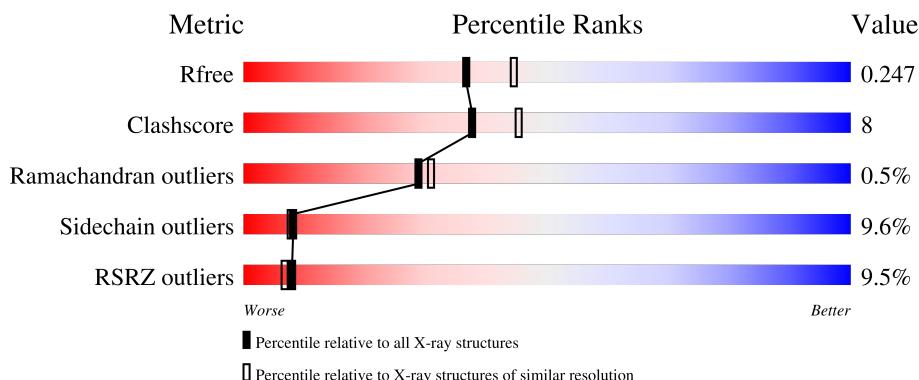
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
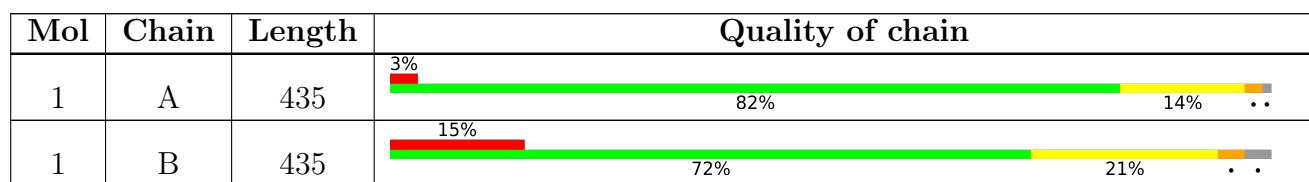
The reported resolution of this entry is 2.20 Å.

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	Percentile Ranks	Value
Rfree		0.247
Clashscore		8
Ramachandran outliers		0.5%
Sidechain outliers		9.6%
RSRZ outliers		9.5%

Worse — Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	435	3% / 82% / 14%
1	B	435	15% / 72% / 21%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6757 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 Isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	5	0	0
			3335	2114	591	617	13			
1	B	420	Total	C	N	O	S	63	0	0
			3260	2069	574	604	13			
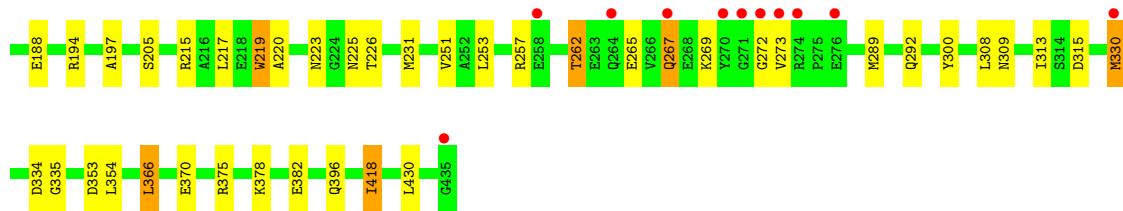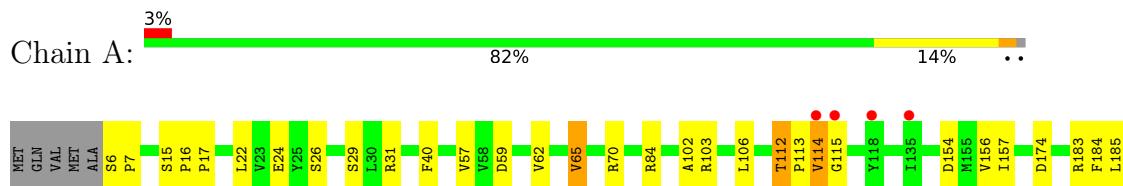
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	37	Total	O	0	0
			37	37		
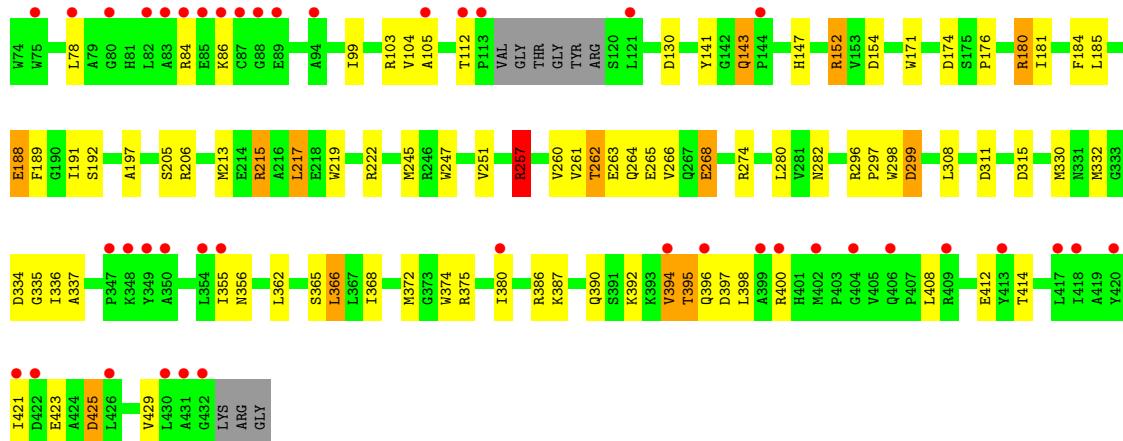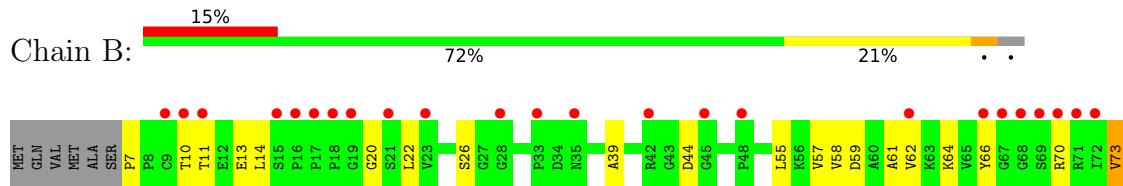
3 Residue-property plots ⓘ

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: Isocitrate dehydrogenase

Chain A:

- Molecule 1: Isocitrate dehydrogenase

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.57Å　　107.57Å　　171.14Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	39.84　–　2.20 39.76　–　2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.84-2.20) 99.9 (39.76-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.225　,　0.251 0.221　,　0.247	Depositor DCC
R_{free} test set	2606 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6757	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.56	0/3405	0.77	5/4619 (0.1%)
1	B	0.51	0/3328	0.74	9/4515 (0.2%)
All	All	0.53	0/6733	0.76	14/9134 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	311	ASP	CB-CG-OD2	8.61	126.05	118.30
1	A	174	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	353	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	334	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	174	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	154	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	59	ASP	CB-CG-OD2	6.01	123.70	118.30
1	A	154	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	397	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	44	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	130	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	257	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	334	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	425	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3335	0	3355	38	0
1	B	3260	0	3277	65	0
2	A	125	0	0	2	0
2	B	37	0	0	2	0
All	All	6757	0	6632	101	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 8.

All (101) 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:152:ARG:HG2	1:B:152:ARG:HH11	1.14	1.13
1:B:104:VAL:HG21	1:B:372:MET:CE	1.81	1.07
1:B:104:VAL:HG21	1:B:372:MET:HE2	1.35	1.04
1:B:104:VAL:HG11	1:B:372:MET:HE3	1.50	0.91
1:A:231:MET:HE2	1:A:309:ASN:HB3	1.54	0.89
1:A:231:MET:CE	1:A:309:ASN:HB3	2.04	0.87
1:B:262:THR:HG22	1:B:265:GLU:H	1.42	0.84
1:A:253:LEU:HD22	1:A:257:ARG:NH1	1.96	0.80
1:B:66:TYR:CD2	1:B:70:ARG:HD2	2.18	0.79
1:B:141:TYR:H	1:B:143:GLN:HE22	1.32	0.77
1:B:104:VAL:CG2	1:B:372:MET:CE	2.61	0.76
1:B:152:ARG:HG2	1:B:152:ARG:NH1	1.93	0.75
1:A:156:VAL:HG21	1:A:219:TRP:CZ2	2.22	0.74
1:A:114:VAL:HG12	1:A:115:GLY:N	2.03	0.73
1:A:6:SER:HB3	1:A:7:PRO:HD3	1.71	0.71
1:B:104:VAL:CG1	1:B:372:MET:HE3	2.19	0.71
1:B:104:VAL:HG11	1:B:372:MET:CE	2.21	0.71
1:B:176:PRO:O	1:B:180:ARG:HG2	1.94	0.68
1:A:223:ASN:ND2	1:A:370:GLU:OE2	2.25	0.67
1:A:103:ARG:HD3	1:A:335:GLY:O	1.97	0.65
1:B:298:TRP:HD1	2:B:453:HOH:O	1.81	0.62
1:B:257:ARG:O	1:B:257:ARG:HD3	1.99	0.62
1:B:66:TYR:CE2	1:B:70:ARG:HD2	2.36	0.61
1:B:55:LEU:O	1:B:59:ASP:HB2	2.02	0.59
1:B:408:LEU:HG	1:B:412:GLU:HB3	1.84	0.59
1:B:104:VAL:HG21	1:B:372:MET:HE1	1.77	0.58
1:A:267:GLN:HA	1:A:272:GLY:HA2	1.84	0.58
1:A:231:MET:HE3	1:A:309:ASN:HB3	1.83	0.58
1:B:70:ARG:NH1	1:B:374:TRP:CD1	2.71	0.58
1:B:10:THR:OG1	1:B:13:GLU:OE2	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:CD	1:A:31:ARG:HH12	2.07	0.57
1:B:104:VAL:CB	1:B:372:MET:CE	2.82	0.57
1:B:143:GLN:H	1:B:143:GLN:NE2	2.03	0.56
1:A:197:ALA:HA	1:B:205:SER:HA	1.87	0.56
1:B:257:ARG:HD3	1:B:257:ARG:C	2.27	0.55
1:B:141:TYR:H	1:B:143:GLN:NE2	2.03	0.55
1:A:57:VAL:HA	1:A:418:ILE:HD11	1.88	0.54
1:B:104:VAL:CB	1:B:372:MET:HE3	2.38	0.54
1:B:57:VAL:HG23	1:B:414:THR:HG23	1.89	0.54
1:A:57:VAL:HA	1:A:418:ILE:CD1	2.38	0.53
1:A:378:LYS:O	1:A:382:GLU:HG3	2.09	0.53
1:B:99:ILE:HG22	1:B:336:ILE:HD11	1.89	0.53
1:A:220:ALA:HA	1:A:225:ASN:HD22	1.73	0.53
1:B:66:TYR:CZ	1:B:70:ARG:NH1	2.77	0.53
1:A:223:ASN:HD21	1:A:370:GLU:CD	2.10	0.52
1:B:143:GLN:H	1:B:143:GLN:HE21	1.56	0.52
1:A:231:MET:SD	1:A:289:MET:HG2	2.50	0.51
1:B:189:PHE:HB2	1:B:191:ILE:HG12	1.93	0.51
1:B:215:ARG:HG3	1:B:332:MET:CE	2.41	0.51
1:A:219:TRP:CD1	1:A:219:TRP:C	2.85	0.50
1:B:104:VAL:CG2	1:B:372:MET:HE2	2.26	0.50
1:B:394:VAL:HG11	1:B:398:LEU:HD12	1.94	0.50
1:B:61:ALA:O	1:B:64:LYS:N	2.45	0.49
1:B:330:MET:HB2	1:B:366:LEU:HD13	1.93	0.49
1:A:65:VAL:HG22	1:A:430:LEU:HD11	1.93	0.49
1:A:308:LEU:C	1:A:308:LEU:HD23	2.34	0.48
1:B:61:ALA:O	1:B:62:VAL:C	2.52	0.47
1:A:262:THR:CG2	1:A:265:GLU:HG3	2.45	0.47
1:B:59:ASP:HA	1:B:62:VAL:HG22	1.96	0.47
1:B:184:PHE:O	1:B:188:GLU:HG3	2.15	0.47
1:B:215:ARG:HG3	1:B:332:MET:HE2	1.96	0.47
1:B:70:ARG:NH1	1:B:374:TRP:CG	2.83	0.47
1:B:262:THR:HG23	2:B:465:HOH:O	2.14	0.47
1:B:213:MET:HG3	1:B:217:LEU:HD22	1.96	0.47
1:B:296:ARG:NE	1:B:299:ASP:OD2	2.33	0.47
1:B:257:ARG:NH2	1:B:265:GLU:OE1	2.45	0.47
1:A:102:ALA:O	1:A:103:ARG:HB2	2.15	0.46
1:B:7:PRO:HB2	1:B:78:LEU:HD11	1.97	0.46
1:A:156:VAL:HG21	1:A:219:TRP:HZ2	1.75	0.46
1:A:262:THR:HG22	1:A:265:GLU:HG3	1.97	0.46
1:B:356:ASN:HA	1:B:395:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG11	1:B:368:ILE:HD13	1.98	0.45
1:A:396:GLN:HG3	2:A:536:HOH:O	2.15	0.45
1:B:152:ARG:HH11	1:B:152:ARG:CG	2.04	0.45
1:A:330:MET:HE3	1:A:366:LEU:HD22	1.98	0.45
1:B:171:TRP:CE3	1:B:181:ILE:HD13	2.52	0.45
1:B:261:VAL:CG1	1:B:266:VAL:HG23	2.47	0.45
1:B:332:MET:HG3	1:B:337:ALA:HB2	1.99	0.44
1:A:157:ILE:HG12	1:A:313:ILE:HG23	1.99	0.44
1:A:253:LEU:HD22	1:A:257:ARG:CZ	2.46	0.44
1:B:103:ARG:HD3	1:B:335:GLY:O	2.17	0.44
1:A:262:THR:HB	1:A:265:GLU:CD	2.39	0.44
1:B:262:THR:HB	1:B:265:GLU:OE2	2.18	0.44
1:A:253:LEU:CD2	1:A:257:ARG:NH1	2.75	0.43
1:B:20:GLY:HA3	1:B:73:VAL:HG21	2.01	0.43
1:B:263:GLU:HG3	1:B:280:LEU:HD11	2.00	0.43
1:B:380:ILE:HG12	1:B:421:ILE:HG12	2.00	0.42
1:A:205:SER:HA	1:B:197:ALA:HA	2.02	0.42
1:A:16:PRO:HA	1:A:17:PRO:HD3	1.91	0.42
1:B:39:ALA:O	1:B:105:ALA:HA	2.20	0.42
1:B:297:PRO:HD2	1:B:298:TRP:CZ3	2.55	0.41
1:B:264:GLN:O	1:B:268:GLU:HB2	2.21	0.41
1:A:84:ARG:NH1	2:A:542:HOH:O	2.37	0.41
1:B:206:ARG:HG3	1:B:247:TRP:CD1	2.56	0.41
1:A:184:PHE:CE1	1:A:188:GLU:HG3	2.56	0.41
1:A:292:GLN:HB3	1:A:300:TYR:CE2	2.56	0.41
1:B:215:ARG:HA	1:B:215:ARG:HD3	1.86	0.41
1:A:112:THR:HA	1:A:113:PRO:HD3	1.79	0.41
1:A:40:PHE:HA	1:A:106:LEU:O	2.22	0.40
1:B:308:LEU:C	1:B:308:LEU:HD23	2.42	0.40
1:B:425:ASP:O	1:B:429:VAL:HG23	2.20	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	428/435 (98%)	408 (95%)	19 (4%)	1 (0%)	47	55
1	B	416/435 (96%)	391 (94%)	22 (5%)	3 (1%)	22	22
All	All	844/870 (97%)	799 (95%)	41 (5%)	4 (0%)	29	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	VAL
1	B	14	LEU
1	B	26	SER
1	B	268	GLU

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	346/350 (99%)	320 (92%)	26 (8%)	13	14
1	B	339/350 (97%)	299 (88%)	40 (12%)	5	4
All	All	685/700 (98%)	619 (90%)	66 (10%)	8	8

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	22	LEU
1	A	26	SER
1	A	29	SER
1	A	62	VAL
1	A	65	VAL
1	A	70	ARG
1	A	112	THR
1	A	183	ARG

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Mol	Chain	Res	Type
1	A	185	LEU
1	A	194	ARG
1	A	215	ARG
1	A	217	LEU
1	A	219	TRP
1	A	226	THR
1	A	251	VAL
1	A	262	THR
1	A	267	GLN
1	A	269	LYS
1	A	273	VAL
1	A	315	ASP
1	A	330	MET
1	A	354	LEU
1	A	366	LEU
1	A	375	ARG
1	A	418	ILE
1	B	11	THR
1	B	22	LEU
1	B	73	VAL
1	B	84	ARG
1	B	86	LYS
1	B	112	THR
1	B	143	GLN
1	B	147	HIS
1	B	152	ARG
1	B	180	ARG
1	B	185	LEU
1	B	188	GLU
1	B	192	SER
1	B	215	ARG
1	B	217	LEU
1	B	219	TRP
1	B	222	ARG
1	B	245	MET
1	B	251	VAL
1	B	257	ARG
1	B	260	VAL
1	B	262	THR
1	B	274	ARG
1	B	282	ASN
1	B	299	ASP

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Mol	Chain	Res	Type
1	B	315	ASP
1	B	355	ILE
1	B	362	LEU
1	B	365	SER
1	B	366	LEU
1	B	375	ARG
1	B	386	ARG
1	B	387	LYS
1	B	390	GLN
1	B	392	LYS
1	B	394	VAL
1	B	395	THR
1	B	396	GLN
1	B	400	ARG
1	B	423	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	147	HIS
1	A	223	ASN
1	A	225	ASN
1	A	292	GLN
1	A	406	GLN
1	B	134	ASN
1	B	143	GLN
1	B	147	HIS
1	B	223	ASN
1	B	225	ASN
1	B	282	ASN
1	B	292	GLN
1	B	390	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, 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(Å²)	Q<0.9
1	A	430/435 (98%)	0.04	15 (3%)	44	42	11, 19, 29, 37	1 (0%)
1	B	420/435 (96%)	0.84	66 (15%)	2	1	14, 19, 24, 27	16 (3%)
All	All	850/870 (97%)	0.43	81 (9%)	8	7	11, 19, 25, 37	17 (2%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	VAL	8.3
1	B	19	GLY	6.4
1	B	66	TYR	5.6
1	B	69	SER	5.6
1	A	272	GLY	5.5
1	B	70	ARG	5.4
1	B	10	THR	5.3
1	B	394	VAL	5.2
1	B	349	TYR	5.1
1	A	270	TYR	5.1
1	B	83	ALA	5.0
1	B	431	ALA	4.9
1	B	420	TYR	4.7
1	B	78	LEU	4.6
1	B	421	ILE	4.6
1	B	15	SER	4.6
1	B	68	GLY	4.5
1	B	67	GLY	4.4
1	B	75	TRP	4.4
1	B	17	PRO	4.2
1	B	400	ARG	4.1
1	B	347	PRO	4.0
1	B	348	LYS	3.9
1	B	432	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	3.8
1	B	413	TYR	3.7
1	B	94	ALA	3.6
1	B	11	THR	3.6
1	B	21	SER	3.6
1	B	88	GLY	3.6
1	B	422	ASP	3.6
1	A	114	VAL	3.5
1	B	28	GLY	3.4
1	B	62	VAL	3.3
1	B	399	ALA	3.3
1	B	71	ARG	3.2
1	B	33	PRO	3.2
1	B	380	ILE	3.2
1	B	406	GLN	3.2
1	B	72	ILE	3.2
1	B	85	GLU	3.2
1	B	16	PRO	3.1
1	B	9	CYS	3.1
1	B	42	ARG	3.1
1	B	354	LEU	3.1
1	B	23	VAL	3.0
1	B	396	GLN	3.0
1	B	144	PRO	3.0
1	B	80	GLY	3.0
1	B	89	GLU	2.9
1	B	84	ARG	2.9
1	B	404	GLY	2.8
1	A	264	GLN	2.7
1	B	418	ILE	2.7
1	B	430	LEU	2.7
1	A	271	GLY	2.7
1	B	35	ASN	2.6
1	A	330	MET	2.6
1	B	402	MET	2.6
1	A	118	TYR	2.6
1	A	435	GLY	2.6
1	A	276	GLU	2.5
1	B	350	ALA	2.5
1	A	135	ILE	2.5
1	B	48	PRO	2.4
1	A	274	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	105	ALA	2.4
1	A	267	GLN	2.4
1	B	355	ILE	2.4
1	A	258	GLU	2.3
1	B	45	GLY	2.2
1	B	121	LEU	2.2
1	B	113	PRO	2.1
1	B	82	LEU	2.1
1	B	112	THR	2.1
1	B	409	ARG	2.1
1	B	86	LYS	2.1
1	B	426	LEU	2.1
1	B	87	CYS	2.0
1	A	115	GLY	2.0
1	B	18	PRO	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 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.