



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:20 AM GMT

PDB ID : 2GPS
Title : Crystal Structure of the Biotin Carboxylase Subunit, E23R mutant, of Acetyl-CoA Carboxylase from Escherichia coli.
Authors : Shen, Y.; Chou, C.Y.; Chang, G.G.; Tong, L.
Deposited on : 2006-04-18
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

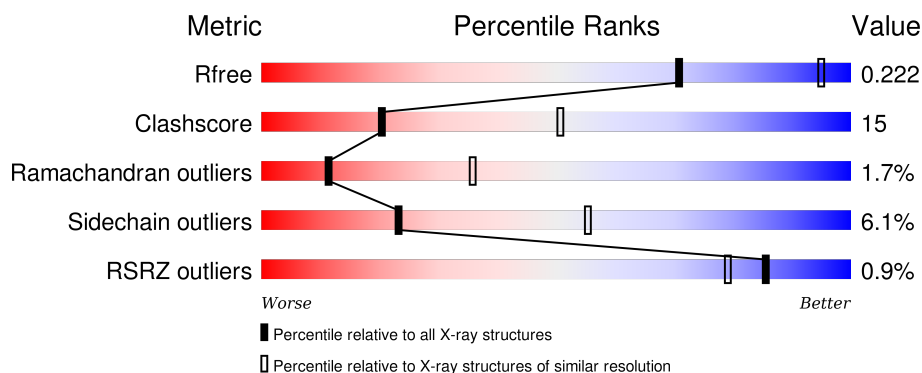
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	469	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 65%, yellow 25%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 65% 25% • 5% </div> </div>
1	B	469	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 63%, yellow 30%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 63% 30% • 5% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6963 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 Biotin carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3450	2174	619	635	22			
1	B	446	Total	C	N	O	S	0	0	0
			3446	2172	618	634	22			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP P24182
A	-18	GLY	-	CLONING ARTIFACT	UNP P24182
A	-17	SER	-	CLONING ARTIFACT	UNP P24182
A	-16	SER	-	CLONING ARTIFACT	UNP P24182
A	-15	HIS	-	EXPRESSION TAG	UNP P24182
A	-14	HIS	-	EXPRESSION TAG	UNP P24182
A	-13	HIS	-	EXPRESSION TAG	UNP P24182
A	-12	HIS	-	EXPRESSION TAG	UNP P24182
A	-11	HIS	-	EXPRESSION TAG	UNP P24182
A	-10	HIS	-	EXPRESSION TAG	UNP P24182
A	-9	SER	-	CLONING ARTIFACT	UNP P24182
A	-8	SER	-	CLONING ARTIFACT	UNP P24182
A	-7	GLY	-	CLONING ARTIFACT	UNP P24182
A	-6	LEU	-	CLONING ARTIFACT	UNP P24182
A	-5	VAL	-	CLONING ARTIFACT	UNP P24182
A	-4	PRO	-	CLONING ARTIFACT	UNP P24182
A	-3	ARG	-	CLONING ARTIFACT	UNP P24182
A	-2	GLY	-	CLONING ARTIFACT	UNP P24182
A	-1	SER	-	CLONING ARTIFACT	UNP P24182
A	0	HIS	-	CLONING ARTIFACT	UNP P24182
A	23	ARG	GLU	ENGINEERED	UNP P24182
B	-19	MET	-	CLONING ARTIFACT	UNP P24182
B	-18	GLY	-	CLONING ARTIFACT	UNP P24182
B	-17	SER	-	CLONING ARTIFACT	UNP P24182
B	-16	SER	-	CLONING ARTIFACT	UNP P24182

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP P24182
B	-14	HIS	-	EXPRESSION TAG	UNP P24182
B	-13	HIS	-	EXPRESSION TAG	UNP P24182
B	-12	HIS	-	EXPRESSION TAG	UNP P24182
B	-11	HIS	-	EXPRESSION TAG	UNP P24182
B	-10	HIS	-	EXPRESSION TAG	UNP P24182
B	-9	SER	-	CLONING ARTIFACT	UNP P24182
B	-8	SER	-	CLONING ARTIFACT	UNP P24182
B	-7	GLY	-	CLONING ARTIFACT	UNP P24182
B	-6	LEU	-	CLONING ARTIFACT	UNP P24182
B	-5	VAL	-	CLONING ARTIFACT	UNP P24182
B	-4	PRO	-	CLONING ARTIFACT	UNP P24182
B	-3	ARG	-	CLONING ARTIFACT	UNP P24182
B	-2	GLY	-	CLONING ARTIFACT	UNP P24182
B	-1	SER	-	CLONING ARTIFACT	UNP P24182
B	0	HIS	-	CLONING ARTIFACT	UNP P24182
B	23	ARG	GLU	ENGINEERED	UNP P24182

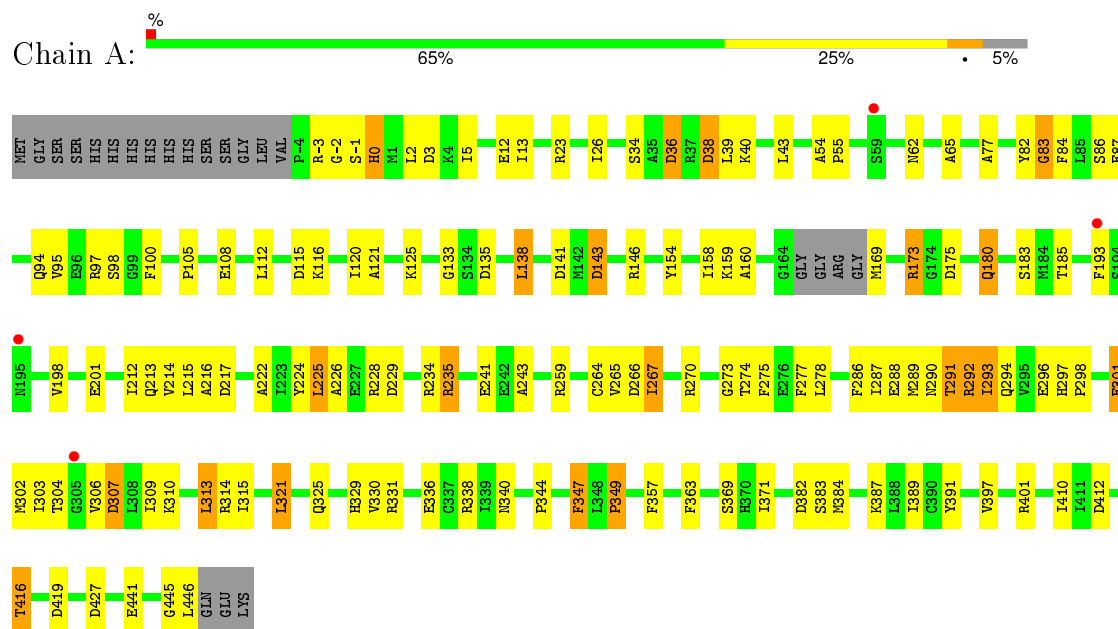
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	38	Total O 38 38	0	0

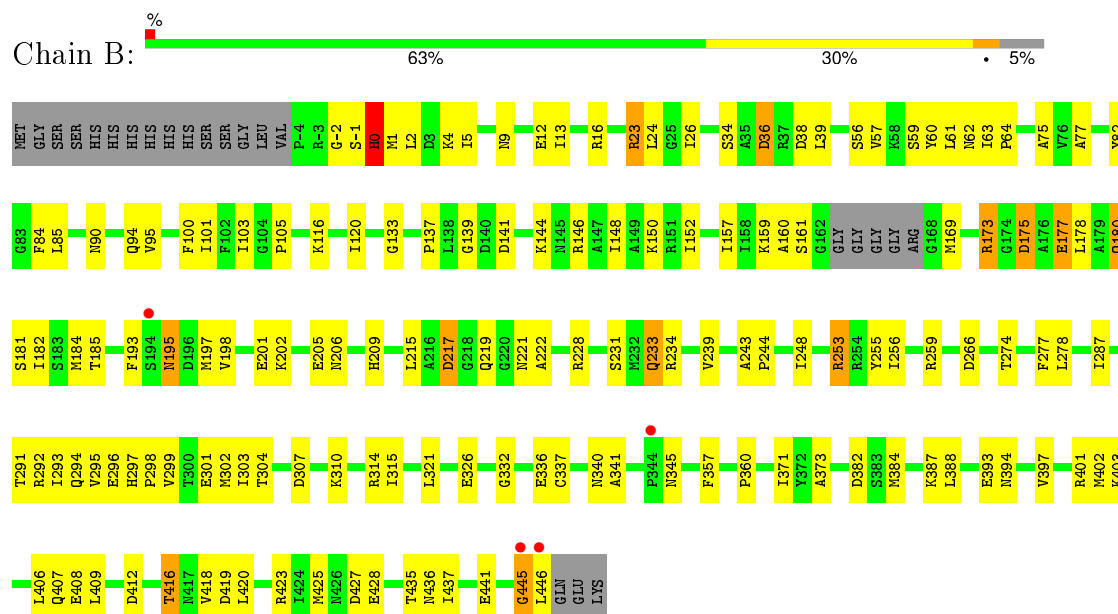
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Biotin carboxylase



• Molecule 1: Biotin carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.93Å 92.62Å 86.60Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.80) 93.7 (29.42-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.201 , 0.260 0.203 , 0.222	Depositor DCC
R_{free} test set	1734 reflections (8.20%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 23678 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6963	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.64	1/3514 (0.0%)	0.87	14/4741 (0.3%)
1	B	0.63	0/3510	0.82	7/4736 (0.1%)
All	All	0.64	1/7024 (0.0%)	0.85	21/9477 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	GLY	C-O	-5.96	1.14	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	GLY	O-C-N	-8.38	109.29	122.70
1	A	217	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	38	ASP	CB-CG-OD2	6.97	124.58	118.30
1	B	141	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	115	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	36	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	412	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	266	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	36	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	266	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	307	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	427	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	135	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	143	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	217	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	38	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	427	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	229	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	412	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	313	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	419	ASP	CB-CG-OD2	5.01	122.81	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	3450	0	3478	99	1
1	B	3446	0	3475	107	0
2	A	29	0	0	1	0
2	B	38	0	0	2	0
All	All	6963	0	6953	202	1

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 15.

All (202) 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:A:298:PRO:HA	1:A:301:GLU:HG3	1.25	1.15
1:B:278:LEU:HG	1:B:287:ILE:HD11	1.31	1.11
1:A:310:LYS:HB3	1:A:314:ARG:NH2	1.86	0.91
1:A:36:ASP:HB3	1:A:39:LEU:CD1	2.02	0.90
1:B:180:GLN:H	1:B:180:GLN:HE21	1.22	0.86
1:A:307:ASP:HB3	1:A:310:LYS:HB2	1.56	0.86
1:A:94:GLN:HG2	1:A:97:ARG:HH21	1.43	0.83
1:A:105:PRO:HG3	1:A:291:THR:HG23	1.63	0.80
1:B:274:THR:OG1	1:B:294:GLN:HG2	1.80	0.80
1:A:278:LEU:HG	1:A:287:ILE:HD11	1.64	0.77
1:A:274:THR:OG1	1:A:294:GLN:HG3	1.85	0.77
1:A:5:ILE:HD12	1:A:26:ILE:HG21	1.68	0.74
1:A:401:ARG:HE	1:B:23:ARG:NH1	1.85	0.73
1:B:310:LYS:HG2	1:B:314:ARG:NH1	2.04	0.73
1:B:-2:GLY:C	1:B:0:HIS:H	1.93	0.72
1:B:373:ALA:HB3	2:B:474:HOH:O	1.90	0.71
1:B:57:VAL:HA	1:B:61:LEU:HD12	1.75	0.69
1:A:401:ARG:HE	1:B:23:ARG:HH12	1.37	0.68
1:B:61:LEU:HA	1:B:85:LEU:HD21	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLY:O	1:A:84:PHE:HB2	1.94	0.67
1:A:274:THR:OG1	1:A:294:GLN:CG	2.42	0.67
1:B:159:LYS:HG2	1:B:169:MET:HG2	1.76	0.67
1:B:116:LYS:O	1:B:120:ILE:HG12	1.94	0.67
1:A:310:LYS:HD3	1:A:314:ARG:NH2	2.11	0.66
1:B:5:ILE:HG13	1:B:26:ILE:HG21	1.77	0.66
1:A:234:ARG:O	1:A:441:GLU:OE1	2.13	0.66
1:B:420:LEU:HA	1:B:423:ARG:HD3	1.78	0.66
1:A:241:GLU:OE2	1:A:336:GLU:OE1	2.14	0.65
1:B:160:ALA:HA	1:B:198:VAL:HG12	1.78	0.64
1:A:291:THR:O	1:A:291:THR:HG22	1.96	0.64
1:B:274:THR:HG21	1:B:294:GLN:HE21	1.63	0.64
1:B:105:PRO:HG3	1:B:291:THR:HB	1.80	0.64
1:A:36:ASP:HB3	1:A:39:LEU:HD12	1.77	0.64
1:B:228:ARG:NH2	1:B:294:GLN:HG3	2.12	0.64
1:B:416:THR:CG2	1:B:418:VAL:HG23	2.29	0.63
1:B:144:LYS:O	1:B:148:ILE:HG13	1.99	0.63
1:B:296:GLU:O	1:B:299:VAL:HG22	1.98	0.63
1:B:274:THR:OG1	1:B:294:GLN:CG	2.47	0.62
1:A:116:LYS:O	1:A:120:ILE:HG12	1.99	0.62
1:A:340:ASN:HD22	1:A:384:MET:HA	1.66	0.61
1:B:340:ASN:HD22	1:B:384:MET:HA	1.66	0.60
1:B:36:ASP:HB3	1:B:39:LEU:HD12	1.83	0.60
1:A:180:GLN:O	1:A:183:SER:HB3	2.00	0.60
1:B:402:MET:HG2	1:B:425:MET:HE3	1.82	0.59
1:A:274:THR:O	1:A:289:MET:HA	2.02	0.59
1:A:121:ALA:O	1:A:125:LYS:HG2	2.02	0.58
1:A:302:MET:CE	1:A:391:TYR:HB2	2.33	0.58
1:A:159:LYS:HG2	1:A:169:MET:HG3	1.86	0.58
1:A:36:ASP:HB3	1:A:39:LEU:HD11	1.83	0.57
1:A:302:MET:HE3	1:A:391:TYR:HB2	1.87	0.57
1:B:16:ARG:NH2	1:B:301:GLU:OE1	2.38	0.56
1:A:298:PRO:HA	1:A:301:GLU:CG	2.17	0.56
1:A:-3:ARG:HD2	1:A:3:ASP:OD2	2.06	0.56
1:B:173:ARG:NH1	1:B:173:ARG:HB3	2.20	0.55
1:A:303:ILE:HG13	1:A:304:THR:HG23	1.86	0.55
1:B:295:VAL:HG12	1:B:387:LYS:HD3	1.89	0.55
1:A:216:ALA:O	1:A:270:ARG:HA	2.07	0.55
1:A:286:PHE:CZ	1:A:288:GLU:HA	2.42	0.54
1:A:307:ASP:CB	1:A:310:LYS:HB2	2.33	0.54
1:B:307:ASP:HB3	1:B:310:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLY:O	1:B:446:LEU:HD12	2.07	0.54
1:A:336:GLU:HG3	1:A:389:ILE:HG13	1.90	0.53
1:B:2:LEU:HD22	1:B:77:ALA:HB2	1.88	0.53
1:B:416:THR:HG22	1:B:418:VAL:H	1.72	0.53
1:B:419:ASP:O	1:B:423:ARG:HG3	2.08	0.53
1:B:416:THR:HG21	1:B:418:VAL:HG23	1.91	0.53
1:B:24:LEU:HD21	1:B:310:LYS:HE2	1.91	0.52
1:B:310:LYS:HG2	1:B:314:ARG:HH12	1.73	0.52
1:B:337:CYS:SG	1:B:425:MET:HE2	2.49	0.52
1:B:4:LYS:HB3	1:B:75:ALA:HA	1.91	0.52
1:B:62:ASN:OD1	1:B:64:PRO:HG2	2.10	0.52
1:A:224:TYR:HE1	1:A:325:GLN:HE21	1.56	0.51
1:B:416:THR:CG2	1:B:418:VAL:H	2.24	0.51
1:B:228:ARG:HH21	1:B:294:GLN:HG3	1.74	0.51
1:B:2:LEU:HD21	1:B:101:ILE:HD12	1.92	0.51
1:A:23:ARG:HH11	1:B:401:ARG:HE	1.58	0.51
1:B:205:GLU:HG2	1:B:206:ASN:OD1	2.10	0.51
1:A:214:VAL:HG22	1:A:273:GLY:O	2.11	0.51
1:A:12:GLU:CD	1:A:387:LYS:HE2	2.31	0.51
1:B:206:ASN:HD22	1:B:436:ASN:ND2	2.09	0.51
1:B:303:ILE:HG13	1:B:304:THR:HG23	1.93	0.51
1:B:217:ASP:OD1	1:B:221:ASN:HB2	2.10	0.51
1:B:-2:GLY:O	1:B:0:HIS:N	2.44	0.51
1:A:62:ASN:HB3	1:A:65:ALA:HB3	1.93	0.50
1:B:248:ILE:HG22	1:B:253:ARG:HG2	1.93	0.50
1:A:83:GLY:O	1:A:84:PHE:CB	2.46	0.50
1:A:87:GLU:HG2	1:A:291:THR:O	2.12	0.50
1:A:344:PRO:HG3	1:A:416:THR:O	2.12	0.50
1:B:357:PHE:CE2	1:B:371:ILE:HD11	2.47	0.49
1:A:310:LYS:HB3	1:A:314:ARG:CZ	2.40	0.49
1:B:221:ASN:HB3	1:B:321:LEU:HD12	1.93	0.49
1:A:0:HIS:O	1:A:0:HIS:CG	2.64	0.49
1:A:310:LYS:HD3	1:A:314:ARG:HH21	1.77	0.49
1:B:315:ILE:HD11	1:B:321:LEU:CD2	2.43	0.49
1:A:154:TYR:N	2:A:475:HOH:O	2.33	0.49
1:A:23:ARG:NH1	1:B:401:ARG:HE	2.11	0.48
1:A:309:ILE:O	1:A:313:LEU:HD22	2.13	0.48
1:A:369:SER:OG	1:A:371:ILE:HG12	2.14	0.48
1:A:290:ASN:HB3	1:A:292:ARG:NH1	2.28	0.48
1:B:-2:GLY:C	1:B:0:HIS:N	2.64	0.48
1:A:234:ARG:NH1	1:A:347:PHE:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ILE:HB	1:B:82:TYR:CE2	2.48	0.48
1:B:137:PRO:HB3	1:B:197:MET:HE3	1.96	0.48
1:A:275:PHE:HB3	1:A:277:PHE:CE1	2.48	0.48
1:A:133:GLY:HA2	1:A:201:GLU:HA	1.96	0.48
1:A:0:HIS:NE2	1:A:26:ILE:HG12	2.29	0.48
1:B:294:GLN:OE1	1:B:294:GLN:HA	2.14	0.48
1:B:12:GLU:CD	1:B:387:LYS:HE2	2.34	0.47
1:A:112:LEU:HD23	1:A:267:ILE:HD11	1.95	0.47
1:B:9:ASN:ND2	1:B:82:TYR:O	2.43	0.47
1:B:360:PRO:HB3	1:B:408:GLU:HB3	1.96	0.47
1:B:402:MET:HG2	1:B:425:MET:CE	2.44	0.47
1:A:146:ARG:CG	1:A:175:ASP:OD1	2.63	0.47
1:B:152:ILE:HG23	1:B:202:LYS:HB2	1.96	0.46
1:B:5:ILE:HG13	1:B:26:ILE:CG2	2.45	0.46
1:A:180:GLN:HE21	1:A:180:GLN:H	1.63	0.46
1:A:13:ILE:HD13	1:A:82:TYR:CE2	2.50	0.46
1:B:90:ASN:HB3	1:B:94:GLN:HE22	1.80	0.46
1:A:36:ASP:HB3	1:A:39:LEU:CG	2.45	0.46
1:B:133:GLY:HA2	1:B:201:GLU:HA	1.96	0.46
1:A:2:LEU:HD22	1:A:77:ALA:HB2	1.96	0.46
1:A:349:PRO:HG3	1:A:383:SER:HB3	1.97	0.46
1:A:264:CYS:O	1:A:267:ILE:HG22	2.16	0.46
1:B:360:PRO:HD3	1:B:409:LEU:HD13	1.96	0.46
1:A:234:ARG:HH21	1:A:235:ARG:HG3	1.81	0.46
1:B:12:GLU:OE2	1:B:387:LYS:HE2	2.16	0.46
1:A:310:LYS:CB	1:A:314:ARG:NH2	2.71	0.46
1:A:158:ILE:O	1:A:169:MET:HA	2.16	0.46
1:A:94:GLN:O	1:A:98:SER:HB2	2.16	0.45
1:B:299:VAL:CG1	1:B:336:GLU:HB2	2.47	0.45
1:B:173:ARG:HG3	1:B:177:GLU:OE1	2.17	0.45
1:A:173:ARG:NH1	1:A:173:ARG:HB3	2.32	0.45
1:B:146:ARG:HG2	1:B:175:ASP:OD1	2.16	0.45
1:B:95:VAL:HG13	1:B:100:PHE:HB2	1.97	0.45
1:A:54:ALA:HB3	1:A:55:PRO:HD3	1.97	0.45
1:B:293:ILE:HD11	1:B:297:HIS:CG	2.52	0.45
1:A:180:GLN:NE2	1:A:180:GLN:H	2.14	0.45
1:B:256:ILE:HD11	1:B:277:PHE:CZ	2.51	0.45
1:B:181:SER:HA	1:B:184:MET:HG3	1.99	0.45
1:B:209:HIS:CD2	1:B:209:HIS:C	2.90	0.45
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.85	0.44
1:A:309:ILE:O	1:A:313:LEU:CD2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:O	1:A:120:ILE:CG1	2.65	0.44
1:A:303:ILE:HG13	1:A:304:THR:N	2.32	0.44
1:A:304:THR:O	1:A:331:ARG:NH1	2.48	0.44
1:A:357:PHE:HA	1:A:410:ILE:O	2.17	0.44
1:B:441:GLU:HB3	1:B:446:LEU:HB2	1.99	0.44
1:B:243:ALA:HA	1:B:244:PRO:C	2.37	0.44
1:A:13:ILE:HD13	1:A:82:TYR:HE2	1.83	0.44
1:B:178:LEU:O	1:B:182:ILE:HG13	2.18	0.44
1:B:161:SER:OG	1:B:197:MET:CE	2.66	0.43
1:A:315:ILE:HD11	1:A:321:LEU:CD2	2.48	0.43
1:A:336:GLU:OE2	1:A:387:LYS:HD2	2.17	0.43
1:A:212:ILE:HG23	1:A:226:ALA:O	2.18	0.43
1:A:141:ASP:OD2	1:A:143:ASP:HB2	2.18	0.43
1:B:420:LEU:O	1:B:423:ARG:HB2	2.18	0.43
1:A:40:LYS:HA	1:A:40:LYS:HD2	1.81	0.43
1:A:296:GLU:OE2	1:A:338:ARG:NH2	2.52	0.43
1:B:36:ASP:HB3	1:B:39:LEU:CD1	2.47	0.43
1:B:388:LEU:HD23	1:B:406:LEU:HD23	2.00	0.43
1:B:297:HIS:N	1:B:298:PRO:CD	2.82	0.42
1:A:228:ARG:HG2	1:A:243:ALA:HB2	2.01	0.42
1:B:77:ALA:HB1	1:B:103:ILE:HD11	2.02	0.42
1:A:146:ARG:HG3	1:A:175:ASP:OD1	2.20	0.42
1:B:403:LYS:HE3	1:B:403:LYS:HB2	1.83	0.42
1:A:95:VAL:HG13	1:A:100:PHE:HB2	2.02	0.42
1:A:274:THR:OG1	1:A:294:GLN:HG2	2.20	0.42
1:B:157:ILE:HD11	1:B:169:MET:HB3	2.02	0.42
1:B:146:ARG:O	1:B:150:LYS:HB2	2.20	0.42
1:B:274:THR:HG1	1:B:294:GLN:HG2	1.78	0.42
1:B:298:PRO:O	1:B:302:MET:HG2	2.18	0.42
1:A:160:ALA:HA	1:A:198:VAL:HG12	2.01	0.42
1:A:215:LEU:O	1:A:222:ALA:HA	2.20	0.42
1:B:307:ASP:HB3	1:B:310:LYS:CB	2.50	0.42
1:B:63:ILE:N	1:B:64:PRO:HD2	2.35	0.42
1:B:293:ILE:HG22	2:B:470:HOH:O	2.19	0.41
1:A:304:THR:C	1:A:331:ARG:HH12	2.24	0.41
1:B:56:SER:HB2	1:B:60:TYR:HB2	2.01	0.41
1:B:82:TYR:C	1:B:82:TYR:CD1	2.94	0.41
1:B:255:TYR:O	1:B:259:ARG:HD3	2.21	0.41
1:B:233:GLN:HA	1:B:239:VAL:HG23	2.03	0.41
1:B:231:SER:O	1:B:437:ILE:HA	2.20	0.41
1:A:38:ASP:HA	1:A:43:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:CD	1:A:314:ARG:NH2	2.81	0.41
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.94	0.41
1:B:418:VAL:O	1:B:419:ASP:C	2.57	0.41
1:A:302:MET:HE2	1:A:391:TYR:HB2	2.03	0.41
1:B:206:ASN:HB3	1:B:436:ASN:HD22	1.85	0.41
1:B:195:ASN:O	1:B:195:ASN:ND2	2.54	0.41
1:A:213:GLN:HG3	1:A:225:LEU:HD12	2.03	0.41
1:A:-1:SER:O	1:A:0:HIS:HB3	2.21	0.40
1:B:394:ASN:OD1	1:B:397:VAL:HG23	2.20	0.40
1:A:293:ILE:HD11	1:A:297:HIS:CG	2.56	0.40
1:A:310:LYS:HB3	1:A:314:ARG:HH21	1.74	0.40
1:A:303:ILE:HD12	1:A:330:VAL:HG13	2.02	0.40
1:B:315:ILE:HD11	1:B:321:LEU:HD21	2.03	0.40
1:B:215:LEU:O	1:B:222:ALA:HA	2.21	0.40
1:B:293:ILE:HG13	1:B:294:GLN:N	2.35	0.40
1:B:297:HIS:N	1:B:298:PRO:HD3	2.36	0.40
1:A:105:PRO:CG	1:A:291:THR:HG23	2.43	0.40
1:B:217:ASP:HA	1:B:315:ILE:CG2	2.52	0.40
1:B:332:GLY:HA2	1:B:393:GLU:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:GLY:O	1:A:173:ARG:NH2[1_655]	2.13	0.07

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	443/469 (94%)	394 (89%)	40 (9%)	9 (2%)	9 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	442/469 (94%)	399 (90%)	37 (8%)	6 (1%)	14	42
All	All	885/938 (94%)	793 (90%)	77 (9%)	15 (2%)	11	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	292	ARG
1	A	306	VAL
1	A	347	PHE
1	B	-1	SER
1	B	0	HIS
1	B	84	PHE
1	B	139	GLY
1	A	235	ARG
1	A	321	LEU
1	A	349	PRO
1	A	382	ASP
1	B	341	ALA
1	A	445	GLY
1	B	445	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/378 (96%)	341 (94%)	20 (6%)	27	59
1	B	361/378 (96%)	337 (93%)	24 (7%)	21	51
All	All	722/756 (96%)	678 (94%)	44 (6%)	23	55

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER

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Mol	Chain	Res	Type
1	A	86	SER
1	A	108	GLU
1	A	138	LEU
1	A	173	ARG
1	A	180	GLN
1	A	185	THR
1	A	193	PHE
1	A	225	LEU
1	A	259	ARG
1	A	265	VAL
1	A	267	ILE
1	A	291	THR
1	A	293	ILE
1	A	301	GLU
1	A	329	HIS
1	A	363	PHE
1	A	397	VAL
1	A	416	THR
1	A	446	LEU
1	B	0	HIS
1	B	1	MET
1	B	23	ARG
1	B	34	SER
1	B	59	SER
1	B	173	ARG
1	B	175	ASP
1	B	177	GLU
1	B	180	GLN
1	B	185	THR
1	B	193	PHE
1	B	195	ASN
1	B	219	GLN
1	B	233	GLN
1	B	234	ARG
1	B	253	ARG
1	B	292	ARG
1	B	326	GLU
1	B	345	ASN
1	B	382	ASP
1	B	407	GLN
1	B	416	THR
1	B	428	GLU

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Mol	Chain	Res	Type
1	B	435	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	41	HIS
1	A	145	ASN
1	A	180	GLN
1	A	206	ASN
1	A	213	GLN
1	A	221	ASN
1	A	290	ASN
1	A	319	GLN
1	A	340	ASN
1	A	404	ASN
1	A	421	GLN
1	B	0	HIS
1	B	94	GLN
1	B	145	ASN
1	B	180	GLN
1	B	195	ASN
1	B	209	HIS
1	B	319	GLN
1	B	340	ASN
1	B	404	ASN
1	B	436	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	447/469 (95%)	-0.17	4 (0%)	85 79	28, 44, 61, 73	2 (0%)
1	B	446/469 (95%)	-0.16	4 (0%)	85 79	23, 45, 61, 68	2 (0%)
All	All	893/938 (95%)	-0.17	8 (0%)	85 79	23, 44, 61, 73	4 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	PHE	4.4
1	B	194	SER	2.8
1	B	446	LEU	2.4
1	A	305	GLY	2.3
1	B	445	GLY	2.1
1	A	195	ASN	2.0
1	B	344	PRO	2.0
1	A	59	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.