



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:18 AM UTC

PDB ID : 2A7K / pdb_00002a7k
Title : carboxymethylproline synthase (CarB) from pectobacterium carotovora, apo enzyme
Authors : Sleeman, M.C.; Sorensen, J.L.; Batchelar, E.T.; McDonough, M.A.; Schofield, C.J.
Deposited on : 2005-07-05
Resolution : 2.24 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

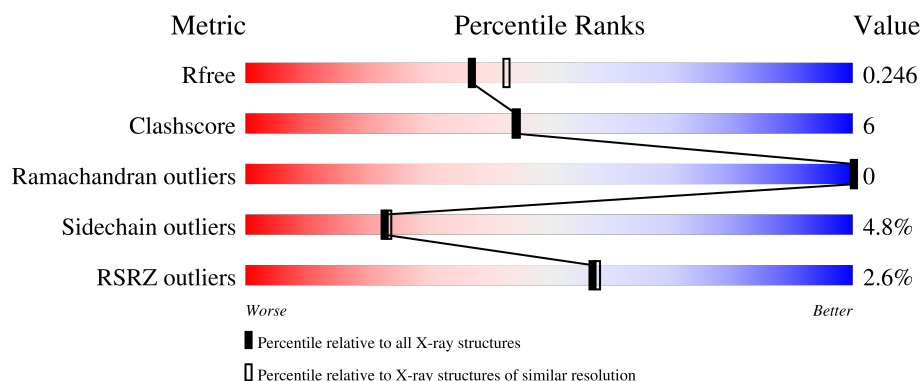
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	250	 3% 77% 15% 8%
1	B	250	 3% 78% 12% 8%
1	C	250	 % 82% 13% 5%
1	D	250	 2% 74% 16% 9%
1	E	250	 2% 75% 18% 6%

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Mol	Chain	Length	Quality of chain
1	F	250	76% 14% • 10%
1	G	250	4% 77% 14% 9%
1	H	250	3% 76% 15% • 8%
1	I	250	3% 77% 13% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16704 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 CarB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1756	1104	305	337	10			
1	B	230	Total	C	N	O	S	0	0	0
			1764	1108	310	336	10			
1	C	238	Total	C	N	O	S	0	0	0
			1833	1152	320	351	10			
1	D	228	Total	C	N	O	S	0	0	0
			1752	1102	305	335	10			
1	E	236	Total	C	N	O	S	0	0	0
			1798	1134	311	343	10			
1	F	226	Total	C	N	O	S	0	0	0
			1745	1097	303	335	10			
1	G	228	Total	C	N	O	S	0	0	0
			1726	1087	302	327	10			
1	H	231	Total	C	N	O	S	0	0	0
			1769	1114	305	340	10			
1	I	228	Total	C	N	O	S	0	0	0
			1755	1105	305	335	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	102	Total	O	0	0
			102	102		
2	C	96	Total	O	0	0
			96	96		
2	D	117	Total	O	0	0
			117	117		
2	E	80	Total	O	0	0
			80	80		

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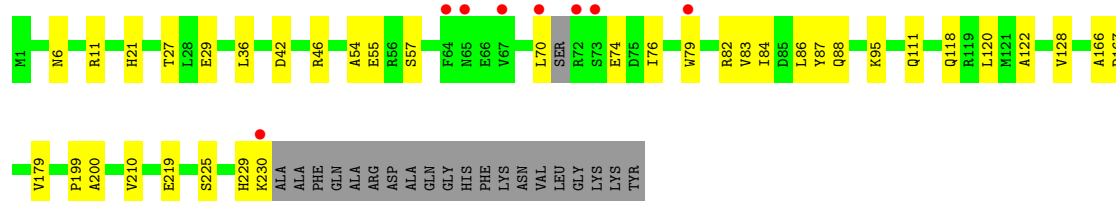
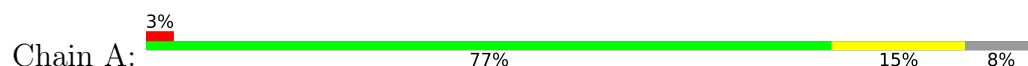
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	83	Total 83	O 83	0	0
2	G	77	Total 77	O 77	0	0
2	H	80	Total 80	O 80	0	0
2	I	89	Total 89	O 89	0	0

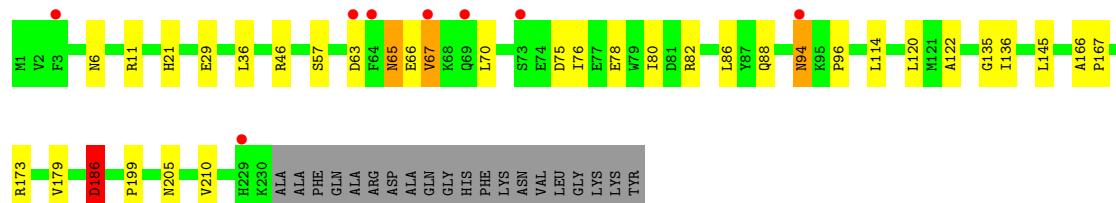
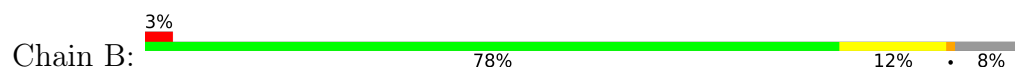
3 Residue-property plots [i](#)

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.

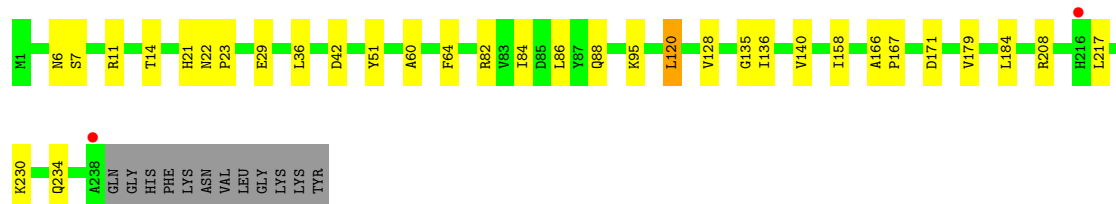
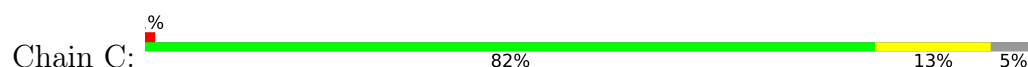
• Molecule 1: CarB



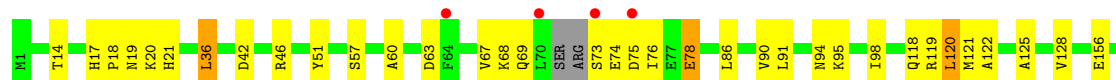
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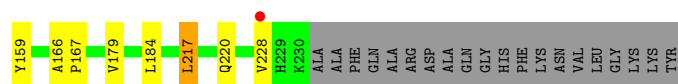


• Molecule 1: CarB

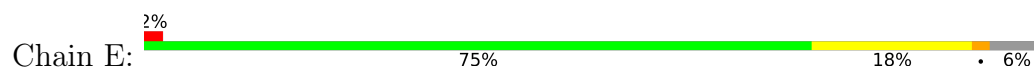


• Molecule 1: CarB

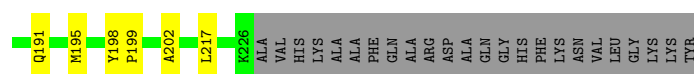




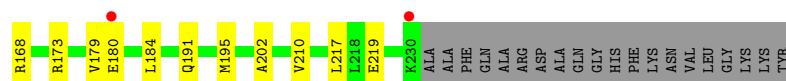
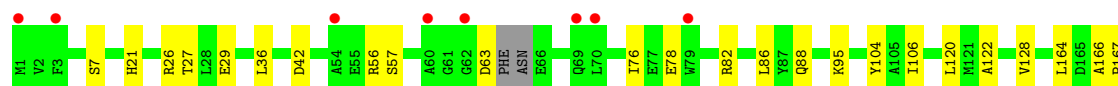
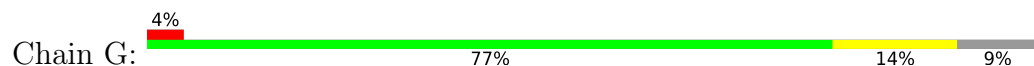
• Molecule 1: CarB



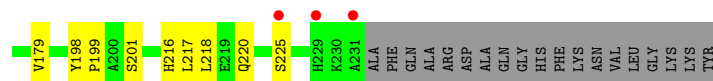
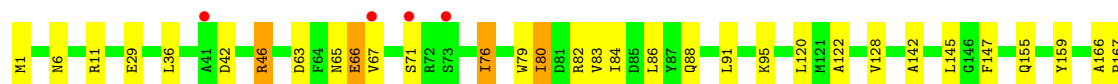
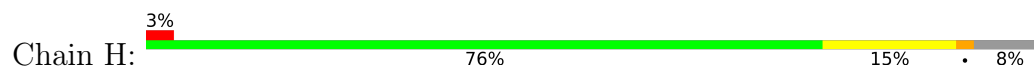
• Molecule 1: CarB



• Molecule 1: CarB

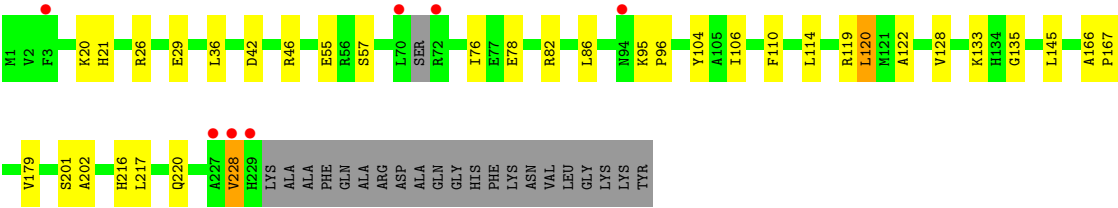


• Molecule 1: CarB



• Molecule 1: CarB





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.21Å 89.86Å 264.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.60 – 2.24 45.60 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.60-2.24) 99.7 (45.60-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 2.24Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0005	Depositor
R, R_{free}	0.185 , 0.238 0.195 , 0.246	Depositor DCC
R_{free} test set	5084 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16704	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.22% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.96	1/1787 (0.1%)	0.96	0/2421
1	B	1.04	3/1796 (0.2%)	1.01	2/2434 (0.1%)
1	C	0.97	1/1867 (0.1%)	0.97	0/2530
1	D	1.03	0/1784	0.99	0/2418
1	E	0.94	1/1832 (0.1%)	0.96	0/2486
1	F	0.91	0/1777	0.94	1/2408 (0.0%)
1	G	0.90	0/1757	0.95	0/2384
1	H	0.93	0/1802	0.98	1/2444 (0.0%)
1	I	0.95	0/1787	1.00	2/2422 (0.1%)
All	All	0.96	6/16189 (0.0%)	0.97	6/21947 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	VAL	CA-CB	6.40	1.62	1.54
1	E	99	ALA	CA-CB	-6.14	1.45	1.53
1	A	210	VAL	CA-CB	5.84	1.61	1.54
1	B	94	ASN	CB-CG	5.53	1.65	1.52
1	B	210	VAL	CA-CB	5.46	1.60	1.54
1	B	136	ILE	CA-CB	5.34	1.60	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	228	VAL	N-CA-C	-11.31	99.30	110.72
1	I	76	ILE	CB-CA-C	-6.78	102.99	112.14
1	B	205	ASN	CB-CA-C	-5.66	101.39	110.79
1	B	186	ASP	N-CA-CB	-5.36	102.25	110.12
1	H	80	ILE	CB-CA-C	-5.26	105.23	111.97
1	F	76	ILE	CB-CA-C	-5.01	105.47	111.88

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	1756	0	1710	22	0
1	B	1764	0	1724	25	0
1	C	1833	0	1793	16	0
1	D	1752	0	1707	29	0
1	E	1798	0	1747	28	0
1	F	1745	0	1710	22	0
1	G	1726	0	1677	15	0
1	H	1769	0	1727	24	0
1	I	1755	0	1716	18	0
2	A	82	0	0	2	0
2	B	102	0	0	3	0
2	C	96	0	0	1	0
2	D	117	0	0	4	0
2	E	80	0	0	0	0
2	F	83	0	0	0	0
2	G	77	0	0	2	0
2	H	80	0	0	4	0
2	I	89	0	0	2	0
All	All	16704	0	15511	187	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 (187) 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:H:46:ARG:HH11	1:H:46:ARG:HG2	1.32	0.94
1:D:17:HIS:HD2	1:D:19:ASN:H	1.14	0.93
1:A:6:ASN:HD21	1:A:11:ARG:HH11	1.17	0.92
1:B:6:ASN:HD21	1:B:11:ARG:HE	1.25	0.84
1:F:4:GLU:OE2	1:F:38:ARG:NH2	2.11	0.84
1:E:225:SER:O	1:E:229:HIS:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:OE1	1:B:82:ARG:HD2	1.83	0.77
1:A:42:ASP:O	1:A:95:LYS:NZ	2.19	0.75
1:D:17:HIS:CD2	1:D:19:ASN:H	2.03	0.73
1:F:29:GLU:OE1	1:F:82:ARG:HD2	1.89	0.72
1:D:156:GLU:HG3	1:F:176:ASN:HD22	1.54	0.72
1:H:29:GLU:OE1	1:H:82:ARG:HD2	1.89	0.72
1:I:20:LYS:HD2	2:I:328:HOH:O	1.92	0.69
1:C:29:GLU:OE1	1:C:82:ARG:HD2	1.95	0.67
1:I:29:GLU:OE2	1:I:82:ARG:NH1	2.27	0.67
1:H:46:ARG:HH11	1:H:46:ARG:CG	2.07	0.66
1:E:225:SER:O	1:E:229:HIS:CD2	2.49	0.65
1:B:6:ASN:ND2	1:B:11:ARG:HE	1.92	0.65
1:I:166:ALA:HB3	1:I:167:PRO:HD3	1.80	0.63
1:E:42:ASP:O	1:E:95:LYS:NZ	2.32	0.62
1:D:94:ASN:ND2	2:D:328:HOH:O	2.32	0.62
1:F:1:MET:HG3	1:F:27:THR:HG22	1.82	0.61
1:H:216:HIS:HB3	2:H:292:HOH:O	2.00	0.61
1:C:42:ASP:O	1:C:95:LYS:NZ	2.34	0.61
1:I:42:ASP:O	1:I:95:LYS:NZ	2.34	0.61
1:G:29:GLU:OE1	1:G:82:ARG:HD2	2.02	0.60
1:E:9:GLU:OE2	1:E:193:HIS:ND1	2.30	0.60
1:E:114:LEU:HD11	1:E:145:LEU:HD13	1.84	0.60
1:B:70:LEU:HB3	1:B:76:ILE:CD1	2.32	0.59
1:H:76:ILE:O	1:H:80:ILE:HG12	2.01	0.59
1:A:74:GLU:OE1	1:A:74:GLU:N	2.31	0.59
1:D:74:GLU:O	1:D:78:GLU:HG3	2.02	0.59
1:C:84:ILE:O	1:C:88:GLN:HG2	2.03	0.59
1:D:17:HIS:CD2	1:D:18:PRO:HD2	2.38	0.58
1:A:11:ARG:NH2	2:A:319:HOH:O	2.37	0.57
1:G:88:GLN:NE2	1:G:219:GLU:OE2	2.33	0.57
1:G:42:ASP:O	1:G:95:LYS:NZ	2.38	0.57
1:B:166:ALA:HB3	1:B:167:PRO:HD3	1.86	0.57
1:D:21:HIS:HA	1:D:57:SER:HB2	1.87	0.56
1:D:68:LYS:NZ	2:D:367:HOH:O	2.23	0.56
1:D:156:GLU:HG3	1:F:176:ASN:ND2	2.20	0.56
1:F:21:HIS:HA	1:F:57:SER:HB2	1.88	0.56
1:H:147:PHE:HB2	1:H:217:LEU:HD22	1.87	0.55
1:A:166:ALA:HB3	1:A:167:PRO:HD3	1.88	0.55
1:D:121:MET:HE3	1:D:125:ALA:HB3	1.88	0.55
1:D:74:GLU:O	1:D:78:GLU:CG	2.56	0.54
1:C:11:ARG:NH2	2:C:330:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:OH	1:A:111:GLN:NE2	2.41	0.54
1:E:73:SER:HB3	1:E:233:PHE:CD2	2.43	0.54
1:E:147:PHE:HB2	1:E:217:LEU:HD22	1.90	0.54
1:H:220:GLN:NE2	2:H:292:HOH:O	2.39	0.53
1:F:87:TYR:OH	1:F:111:GLN:NE2	2.42	0.53
1:E:84:ILE:O	1:E:88:GLN:HG2	2.09	0.53
1:B:114:LEU:HD11	1:B:145:LEU:HD13	1.91	0.52
1:A:6:ASN:HD21	1:A:11:ARG:NH1	1.98	0.52
1:C:230:LYS:O	1:C:234:GLN:HG3	2.10	0.52
1:I:216:HIS:CD2	1:I:220:GLN:NE2	2.78	0.52
1:H:46:ARG:HG2	1:H:46:ARG:NH1	2.12	0.51
1:G:202:ALA:HB3	2:H:270:HOH:O	2.11	0.51
1:B:65:ASN:OD1	1:B:65:ASN:N	2.43	0.51
1:E:166:ALA:HB3	1:E:167:PRO:HD3	1.93	0.51
1:E:20:LYS:H	1:E:20:LYS:CD	2.22	0.51
1:E:201:SER:O	1:E:205:ASN:ND2	2.43	0.51
1:D:17:HIS:HD2	1:D:19:ASN:N	1.95	0.50
1:D:74:GLU:H	1:D:74:GLU:CD	2.18	0.50
1:D:217:LEU:HA	1:D:220:GLN:HE21	1.76	0.50
1:E:29:GLU:OE1	1:E:82:ARG:HD2	2.12	0.50
1:F:70:LEU:HB3	1:F:76:ILE:HD13	1.93	0.50
1:F:120:LEU:N	1:F:120:LEU:HD23	2.26	0.50
1:C:179:VAL:HG21	1:C:184:LEU:HA	1.93	0.50
1:E:68:LYS:HE2	1:E:136:ILE:HD11	1.94	0.50
1:I:120:LEU:HD23	1:I:120:LEU:N	2.25	0.50
1:E:210:VAL:HG13	1:F:154:MET:HE1	1.93	0.50
1:D:98:ILE:HD13	1:D:118:GLN:HB2	1.93	0.50
1:A:79:TRP:O	1:A:83:VAL:HG23	2.12	0.49
1:D:119:ARG:NH2	2:D:348:HOH:O	2.41	0.49
1:G:166:ALA:HB3	1:G:167:PRO:HD3	1.94	0.49
1:F:42:ASP:O	1:F:95:LYS:NZ	2.45	0.49
1:B:173:ARG:NH2	1:C:171:ASP:OD2	2.44	0.49
1:G:195:MET:HE3	1:H:159:TYR:HB3	1.95	0.48
1:H:46:ARG:CG	1:H:46:ARG:NH1	2.71	0.48
1:I:114:LEU:HD11	1:I:145:LEU:HD13	1.95	0.48
1:A:46:ARG:NH1	1:A:200:ALA:HB2	2.28	0.48
1:G:122:ALA:HA	1:G:179:VAL:O	2.13	0.48
1:H:198:TYR:CD1	1:I:133:LYS:HA	2.49	0.48
1:C:120:LEU:N	1:C:120:LEU:HD23	2.29	0.47
1:E:21:HIS:HA	1:E:57:SER:HB2	1.96	0.47
1:A:88:GLN:NE2	1:A:219:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ALA:HA	1:F:179:VAL:O	2.15	0.47
1:D:122:ALA:HA	1:D:179:VAL:O	2.14	0.47
1:F:27:THR:HG21	2:I:312:HOH:O	2.13	0.47
1:F:156:GLU:OE1	1:F:172:TYR:OH	2.18	0.47
1:H:42:ASP:O	1:H:95:LYS:NZ	2.48	0.47
1:H:155:GLN:NE2	2:H:290:HOH:O	2.45	0.47
1:B:94:ASN:HA	2:B:321:HOH:O	2.15	0.47
1:F:166:ALA:HB3	1:F:167:PRO:HD3	1.97	0.47
1:G:173:ARG:HG3	2:G:285:HOH:O	2.15	0.47
1:A:118:GLN:NE2	2:A:320:HOH:O	2.47	0.46
1:H:63:ASP:HB3	1:H:66:GLU:HB3	1.97	0.46
1:C:166:ALA:HB3	1:C:167:PRO:HD3	1.97	0.46
1:C:6:ASN:OD1	1:C:11:ARG:HD3	2.16	0.46
1:D:179:VAL:HG21	1:D:184:LEU:HA	1.96	0.46
1:E:72:ARG:O	1:E:75:ASP:HB2	2.15	0.46
1:H:166:ALA:HB3	1:H:167:PRO:HD3	1.96	0.46
1:D:20:LYS:NZ	1:D:21:HIS:NE2	2.61	0.46
1:D:120:LEU:HD23	1:D:120:LEU:N	2.31	0.46
1:I:119:ARG:C	1:I:120:LEU:HD23	2.41	0.46
1:A:29:GLU:OE2	1:A:82:ARG:NH1	2.48	0.45
1:A:229:HIS:O	1:A:230:LYS:CB	2.65	0.45
1:B:21:HIS:HA	1:B:57:SER:HB2	1.98	0.45
1:I:21:HIS:HA	1:I:57:SER:HB2	1.98	0.45
1:A:70:LEU:HD13	1:A:76:ILE:HA	1.97	0.45
1:G:179:VAL:HG21	1:G:184:LEU:HA	1.96	0.45
1:A:199:PRO:HG2	1:B:135:GLY:HA3	1.98	0.45
1:H:91:LEU:HD12	1:H:218:LEU:HD12	1.99	0.45
1:B:67:VAL:HA	1:B:70:LEU:HB2	1.99	0.45
1:C:64:PHE:CD1	1:C:136:ILE:HG13	2.51	0.45
1:G:179:VAL:CG2	1:G:184:LEU:HA	2.47	0.45
1:B:46:ARG:O	1:B:96:PRO:HD2	2.16	0.45
1:B:76:ILE:O	1:B:80:ILE:HG12	2.17	0.45
1:D:217:LEU:O	1:D:217:LEU:HG	2.14	0.44
1:H:6:ASN:OD1	1:H:11:ARG:NH1	2.48	0.44
1:I:104:TYR:HB3	1:I:106:ILE:HG13	1.98	0.44
1:D:42:ASP:O	1:D:95:LYS:NZ	2.51	0.44
1:B:70:LEU:HB3	1:B:76:ILE:HD13	2.00	0.44
1:C:217:LEU:O	1:C:217:LEU:HG	2.08	0.44
1:D:63:ASP:O	1:D:67:VAL:HG23	2.18	0.44
1:H:199:PRO:HG2	1:I:135:GLY:HA3	2.00	0.44
1:B:122:ALA:HA	1:B:179:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:LEU:O	1:E:217:LEU:HG	2.08	0.44
1:H:122:ALA:HA	1:H:179:VAL:O	2.18	0.44
1:C:22:ASN:N	1:C:23:PRO:CD	2.81	0.43
1:A:29:GLU:OE1	1:A:82:ARG:HD2	2.17	0.43
1:E:20:LYS:H	1:E:20:LYS:HD3	1.83	0.43
1:E:122:ALA:HA	1:E:179:VAL:O	2.18	0.43
1:I:110:PHE:C	1:I:110:PHE:CD1	2.95	0.43
1:I:29:GLU:CD	1:I:82:ARG:HH11	2.26	0.43
1:F:1:MET:HE1	1:F:17:HIS:CD2	2.54	0.43
1:G:21:HIS:HA	1:G:57:SER:HB2	2.00	0.43
1:B:70:LEU:HD22	1:B:75:ASP:HB3	2.00	0.43
1:E:104:TYR:HB3	1:E:106:ILE:HG13	2.01	0.43
1:B:186:ASP:OD1	2:B:352:HOH:O	2.21	0.43
1:H:84:ILE:O	1:H:88:GLN:HG2	2.19	0.43
1:A:46:ARG:HH12	1:A:200:ALA:HB2	1.85	0.42
1:A:54:ALA:O	1:A:55:GLU:HB2	2.19	0.42
1:B:186:ASP:HB3	2:B:289:HOH:O	2.19	0.42
1:H:63:ASP:O	1:H:67:VAL:HG23	2.18	0.42
1:F:147:PHE:HB2	1:F:217:LEU:HD22	2.01	0.42
1:I:46:ARG:O	1:I:96:PRO:HD2	2.19	0.42
1:I:122:ALA:HA	1:I:179:VAL:O	2.20	0.42
1:E:120:LEU:HD23	1:E:120:LEU:N	2.34	0.42
2:D:277:HOH:O	1:F:202:ALA:HB3	2.19	0.42
1:F:40:ASN:HA	1:F:95:LYS:HE3	2.02	0.42
1:D:36:LEU:HD21	1:D:90:VAL:HG22	2.02	0.42
1:E:156:GLU:OE1	1:E:172:TYR:OH	2.27	0.42
1:H:79:TRP:O	1:H:83:VAL:HG23	2.19	0.42
1:F:29:GLU:O	1:F:33:LYS:HG3	2.20	0.42
1:C:14:THR:HA	1:C:51:TYR:O	2.20	0.42
1:B:199:PRO:HG2	1:C:135:GLY:HA3	2.01	0.42
1:I:110:PHE:C	1:I:110:PHE:HD1	2.28	0.42
1:E:78:GLU:O	1:E:82:ARG:HG3	2.20	0.41
1:G:63:ASP:OD1	1:G:63:ASP:C	2.63	0.41
1:B:63:ASP:CB	1:B:66:GLU:OE1	2.69	0.41
1:E:73:SER:HB3	1:E:233:PHE:CG	2.55	0.41
1:E:73:SER:C	1:E:75:ASP:N	2.78	0.41
1:G:104:TYR:HB3	1:G:106:ILE:HG13	2.03	0.41
1:A:84:ILE:O	1:A:88:GLN:HG2	2.20	0.41
1:B:114:LEU:CD1	1:B:145:LEU:HD13	2.50	0.41
1:D:166:ALA:HB3	1:D:167:PRO:HD3	2.02	0.41
1:A:122:ALA:HA	1:A:179:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:HIS:HB3	1:C:60:ALA:HB2	2.02	0.41
1:B:88:GLN:HA	1:B:88:GLN:OE1	2.21	0.41
1:D:21:HIS:HB3	1:D:60:ALA:HB2	2.03	0.41
1:D:73:SER:C	1:D:75:ASP:N	2.77	0.41
1:H:80:ILE:HD12	1:H:225:SER:OG	2.21	0.41
1:A:21:HIS:HA	1:A:57:SER:HB2	2.03	0.41
1:D:159:TYR:HB3	1:F:195:MET:HE3	2.04	0.40
1:E:63:ASP:OD2	1:E:66:GLU:N	2.54	0.40
1:E:77:GLU:HG3	1:E:226:LYS:HD3	2.01	0.40
1:G:210:VAL:HG22	1:H:142:ALA:HB1	2.02	0.40
1:B:29:GLU:OE2	1:B:82:ARG:NH1	2.55	0.40
1:E:180:GLU:N	1:E:180:GLU:OE1	2.54	0.40
2:G:268:HOH:O	1:I:202:ALA:HB3	2.21	0.40
1:D:14:THR:HA	1:D:51:TYR:O	2.22	0.40
1:G:164:LEU:HD22	1:G:168:ARG:HG2	2.03	0.40
1:F:198:TYR:O	1:F:199:PRO:C	2.64	0.40
1:A:199:PRO:HG2	1:B:135:GLY:CA	2.52	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	225/250 (90%)	220 (98%)	5 (2%)	0	100	100
1	B	228/250 (91%)	221 (97%)	7 (3%)	0	100	100
1	C	236/250 (94%)	232 (98%)	4 (2%)	0	100	100
1	D	224/250 (90%)	219 (98%)	5 (2%)	0	100	100
1	E	234/250 (94%)	230 (98%)	4 (2%)	0	100	100
1	F	224/250 (90%)	221 (99%)	3 (1%)	0	100	100
1	G	224/250 (90%)	219 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	229/250 (92%)	223 (97%)	6 (3%)	0	100	100
1	I	224/250 (90%)	221 (99%)	3 (1%)	0	100	100
All	All	2048/2250 (91%)	2006 (98%)	42 (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	185/205 (90%)	179 (97%)	6 (3%)	34	40
1	B	186/205 (91%)	179 (96%)	7 (4%)	29	34
1	C	194/205 (95%)	187 (96%)	7 (4%)	31	36
1	D	186/205 (91%)	175 (94%)	11 (6%)	18	16
1	E	188/205 (92%)	178 (95%)	10 (5%)	20	20
1	F	187/205 (91%)	182 (97%)	5 (3%)	39	47
1	G	180/205 (88%)	167 (93%)	13 (7%)	13	10
1	H	188/205 (92%)	176 (94%)	12 (6%)	16	14
1	I	187/205 (91%)	177 (95%)	10 (5%)	20	20
All	All	1681/1845 (91%)	1600 (95%)	81 (5%)	23	23

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	36	LEU
1	A	86	LEU
1	A	120	LEU
1	A	128	VAL
1	A	225	SER
1	B	36	LEU
1	B	65	ASN

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Mol	Chain	Res	Type
1	B	67	VAL
1	B	78	GLU
1	B	86	LEU
1	B	120	LEU
1	B	186	ASP
1	C	7	SER
1	C	36	LEU
1	C	86	LEU
1	C	120	LEU
1	C	128	VAL
1	C	158	ILE
1	C	208	ARG
1	D	36	LEU
1	D	46	ARG
1	D	69	GLN
1	D	76	ILE
1	D	78	GLU
1	D	86	LEU
1	D	91	LEU
1	D	120	LEU
1	D	128	VAL
1	D	217	LEU
1	D	228	VAL
1	E	3	PHE
1	E	20	LYS
1	E	36	LEU
1	E	43	ASP
1	E	55	GLU
1	E	70	LEU
1	E	77	GLU
1	E	86	LEU
1	E	120	LEU
1	E	180	GLU
1	F	36	LEU
1	F	78	GLU
1	F	120	LEU
1	F	128	VAL
1	F	191	GLN
1	G	7	SER
1	G	26	ARG
1	G	27	THR
1	G	36	LEU

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Mol	Chain	Res	Type
1	G	56	ARG
1	G	76	ILE
1	G	78	GLU
1	G	86	LEU
1	G	120	LEU
1	G	128	VAL
1	G	180	GLU
1	G	191	GLN
1	G	217	LEU
1	H	1	MET
1	H	36	LEU
1	H	46	ARG
1	H	65	ASN
1	H	66	GLU
1	H	71	SER
1	H	76	ILE
1	H	86	LEU
1	H	120	LEU
1	H	128	VAL
1	H	145	LEU
1	H	201	SER
1	I	26	ARG
1	I	36	LEU
1	I	55	GLU
1	I	78	GLU
1	I	86	LEU
1	I	120	LEU
1	I	128	VAL
1	I	201	SER
1	I	217	LEU
1	I	228	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	111	GLN
1	A	118	GLN
1	A	126	ASN
1	A	177	GLN
1	A	191	GLN
1	B	6	ASN

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Mol	Chain	Res	Type
1	B	94	ASN
1	B	177	GLN
1	D	17	HIS
1	D	69	GLN
1	D	94	ASN
1	D	134	HIS
1	D	220	GLN
1	E	94	ASN
1	E	118	GLN
1	E	229	HIS
1	F	111	GLN
1	F	216	HIS
1	F	220	GLN
1	G	229	HIS
1	H	94	ASN
1	H	205	ASN
1	I	65	ASN
1	I	118	GLN
1	I	134	HIS
1	I	177	GLN
1	I	191	GLN
1	I	216	HIS
1	I	220	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	229/250 (91%)	-0.04	8 (3%)	47	46	21, 34, 63, 84	0
1	B	230/250 (92%)	-0.04	8 (3%)	47	46	19, 31, 68, 92	0
1	C	238/250 (95%)	-0.13	2 (0%)	82	84	16, 34, 52, 69	1 (0%)
1	D	228/250 (91%)	-0.12	5 (2%)	62	64	19, 30, 58, 78	0
1	E	236/250 (94%)	0.01	6 (2%)	58	59	21, 36, 66, 82	0
1	F	226/250 (90%)	-0.04	1 (0%)	88	90	23, 38, 55, 72	0
1	G	228/250 (91%)	0.16	10 (4%)	39	37	21, 39, 65, 96	1 (0%)
1	H	231/250 (92%)	0.17	7 (3%)	52	52	21, 39, 76, 99	0
1	I	228/250 (91%)	-0.05	7 (3%)	51	51	19, 34, 56, 68	0
All	All	2074/2250 (92%)	-0.01	54 (2%)	57	58	16, 35, 63, 99	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	228	VAL	4.2
1	A	72	ARG	4.2
1	H	231	ALA	3.9
1	G	69	GLN	3.8
1	G	230	LYS	3.8
1	D	73	SER	3.6
1	G	70	LEU	3.5
1	B	63	ASP	3.5
1	E	236	ARG	3.4
1	A	65	ASN	3.3
1	D	228	VAL	3.3
1	B	73	SER	3.3
1	D	70	LEU	3.2
1	B	67	VAL	3.2
1	B	229	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	64	PHE	3.1
1	G	60	ALA	3.0
1	A	67	VAL	2.9
1	B	94	ASN	2.9
1	A	64	PHE	2.9
1	I	227	ALA	2.8
1	G	1	MET	2.7
1	E	72	ARG	2.7
1	F	64	PHE	2.7
1	G	180	GLU	2.7
1	I	72	ARG	2.7
1	A	79	TRP	2.7
1	C	216	HIS	2.6
1	C	238	ALA	2.5
1	H	41	ALA	2.5
1	G	79	TRP	2.5
1	E	73	SER	2.4
1	H	71	SER	2.4
1	D	75	ASP	2.4
1	H	67	VAL	2.3
1	A	73	SER	2.3
1	I	229	HIS	2.3
1	G	62	GLY	2.3
1	A	70	LEU	2.2
1	B	3	PHE	2.2
1	E	233	PHE	2.2
1	H	73	SER	2.2
1	I	3	PHE	2.2
1	G	54	ALA	2.2
1	E	70	LEU	2.2
1	D	64	PHE	2.2
1	A	230	LYS	2.2
1	H	229	HIS	2.2
1	E	74	GLU	2.1
1	I	70	LEU	2.1
1	I	94	ASN	2.0
1	G	3	PHE	2.0
1	H	225	SER	2.0
1	B	69	GLN	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.