



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 PM UTC

PDB ID : 8XVN / pdb_00008xvn
Title : Short-chain dehydrogenase/reductase6 (SDR6) from Antrodia camphorata
Authors : Zhang, Y.Q.; Zhang, M.; Ye, M.
Deposited on : 2024-01-15
Resolution : 2.00 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:

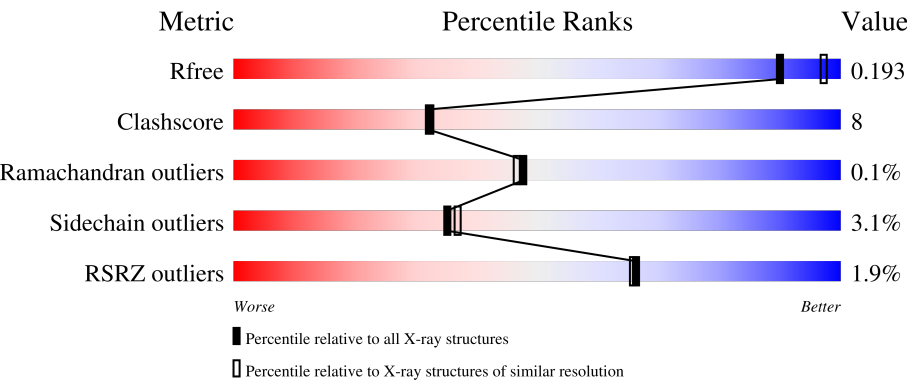
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	270	0.1% 71% 11% • 16%
1	B	270	2% 66% 17% 16%
1	C	270	2% 71% 13% 16%
1	D	270	0.1% 73% 10% • 16%
1	E	270	0.1% 74% 9% • 16%

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Mol	Chain	Length	Quality of chain
1	F	270	% 73% 10% 16%
1	G	270	2% 70% 16% • 14%
1	H	270	2% 69% 15% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14570 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 Short-chain dehydrogenases/reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1663	1050	292	313	8			
1	B	227	Total	C	N	O	S	0	0	0
			1671	1055	293	315	8			
1	C	228	Total	C	N	O	S	0	0	0
			1666	1052	290	316	8			
1	D	227	Total	C	N	O	S	0	0	0
			1671	1054	293	316	8			
1	E	227	Total	C	N	O	S	0	0	0
			1670	1055	292	315	8			
1	F	227	Total	C	N	O	S	0	0	0
			1671	1054	293	316	8			
1	G	232	Total	C	N	O	S	0	0	0
			1705	1080	297	320	8			
1	H	227	Total	C	N	O	S	0	0	0
			1661	1046	293	314	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	155	Total	O	0	0
			155	155		
2	B	149	Total	O	0	0
			149	149		
2	C	162	Total	O	0	0
			162	162		
2	D	148	Total	O	0	0
			148	148		
2	E	159	Total	O	0	0
			159	159		
2	F	145	Total	O	0	0
			145	145		

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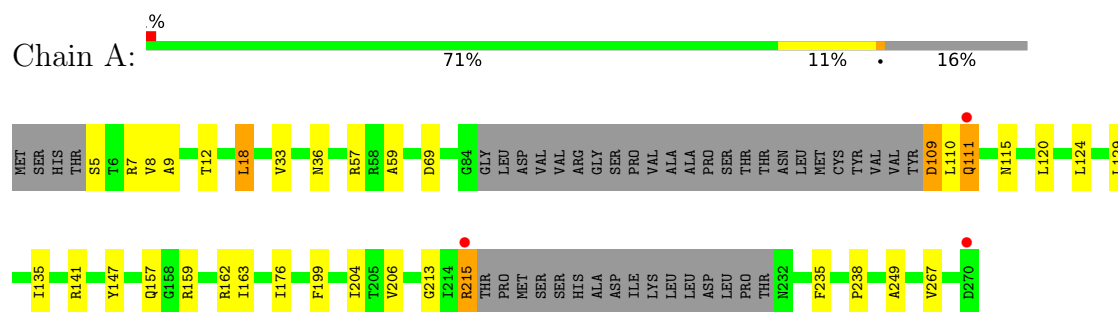
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	151	Total 151	O 151	0	0
2	H	123	Total 123	O 123	0	0

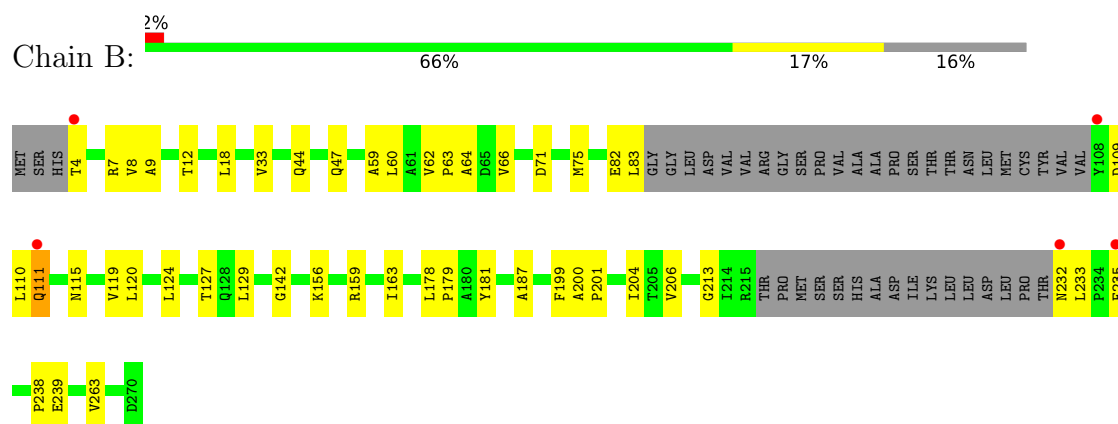
3 Residue-property plots [i](#)

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.

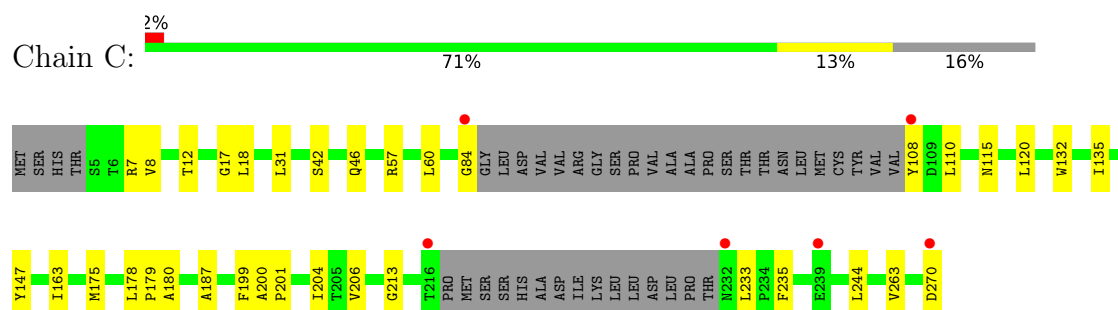
- Molecule 1: Short-chain dehydrogenases/reductase



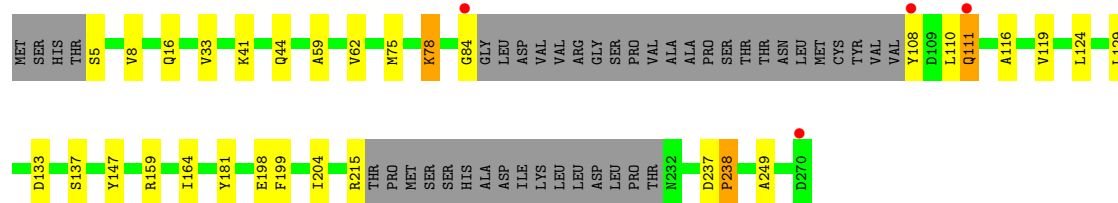
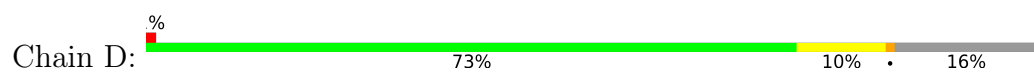
- Molecule 1: Short-chain dehydrogenases/reductase



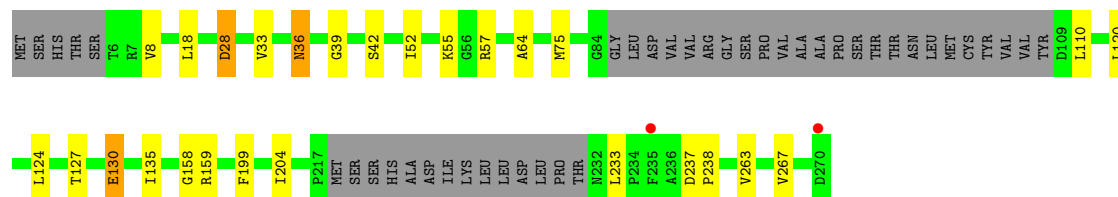
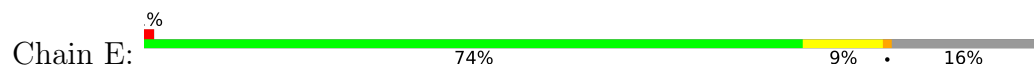
- Molecule 1: Short-chain dehydrogenases/reductase



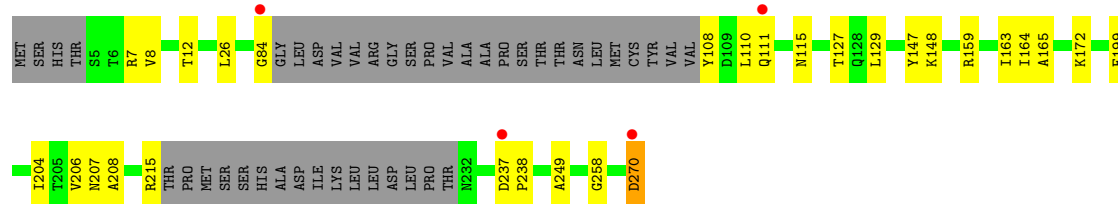
- Molecule 1: Short-chain dehydrogenases/reductase



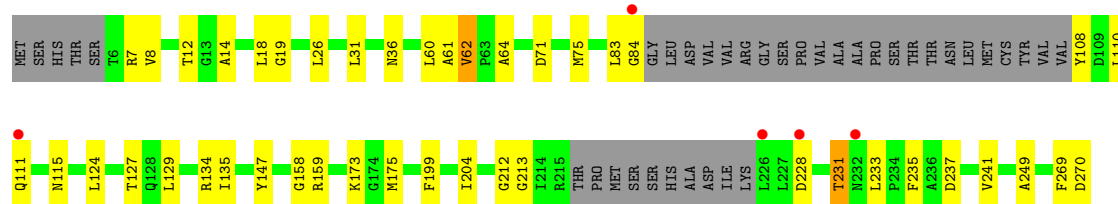
- Molecule 1: Short-chain dehydrogenases/reductase



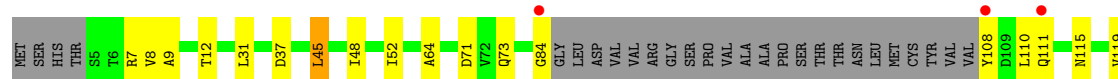
- Molecule 1: Short-chain dehydrogenases/reductase

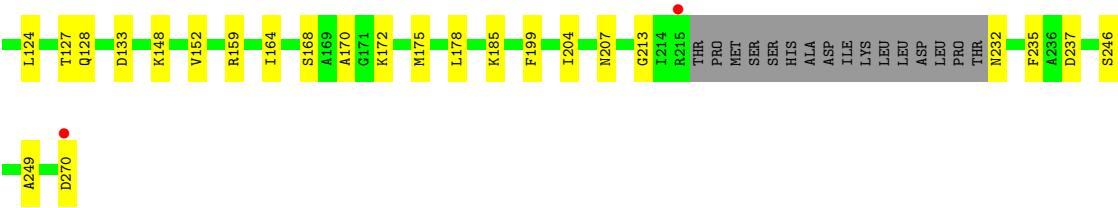


- Molecule 1: Short-chain dehydrogenases/reductase



- Molecule 1: Short-chain dehydrogenases/reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.41Å 133.46Å 94.22Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	39.12 – 2.00 39.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.8 (39.12-2.00) 89.9 (39.12-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.164 , 0.192 0.166 , 0.193	Depositor DCC
R_{free} test set	5018 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14570	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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	1.12	0/1682	1.34	2/2277 (0.1%)
1	B	1.11	1/1690 (0.1%)	1.35	4/2289 (0.2%)
1	C	1.11	0/1685	1.36	0/2283
1	D	1.11	2/1690 (0.1%)	1.36	1/2288 (0.0%)
1	E	1.13	0/1690	1.38	2/2290 (0.1%)
1	F	1.11	0/1690	1.36	0/2288
1	G	1.08	0/1725	1.35	3/2338 (0.1%)
1	H	1.08	0/1679	1.37	0/2274
All	All	1.11	3/13531 (0.0%)	1.36	12/18327 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	137	SER	C-O	-5.67	1.17	1.24
1	D	238	PRO	C-O	-5.44	1.16	1.24
1	B	63	PRO	C-O	-5.00	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	130	GLU	CB-CG-CD	7.73	125.75	112.60
1	E	267	VAL	N-CA-C	-5.73	106.64	111.56
1	G	212	GLY	CA-C-O	-5.60	116.43	121.47
1	D	237	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	109	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	267	VAL	N-CA-C	-5.46	106.37	111.45
1	B	83	LEU	CA-C-O	-5.45	111.53	120.80
1	G	135	ILE	CA-C-O	-5.39	115.45	121.17
1	A	109	ASP	CA-CB-CG	5.33	117.93	112.60
1	G	237	ASP	CB-CA-C	5.31	117.81	109.37
1	B	239	GLU	CB-CG-CD	5.30	121.61	112.60
1	B	263	VAL	CB-CA-C	5.22	117.65	111.59

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	1663	0	1705	36	0
1	B	1671	0	1711	27	0
1	C	1666	0	1694	20	0
1	D	1671	0	1709	31	0
1	E	1670	0	1710	24	0
1	F	1671	0	1709	25	0
1	G	1705	0	1749	33	0
1	H	1661	0	1698	33	0
2	A	155	0	0	1	0
2	B	149	0	0	1	0
2	C	162	0	0	0	0
2	D	148	0	0	2	0
2	E	159	0	0	4	0
2	F	145	0	0	2	0
2	G	151	0	0	2	0
2	H	123	0	0	4	0
All	All	14570	0	13685	217	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 (217) 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:F:111:GLN:OE1	1:F:249:ALA:HB1	1.51	1.10
1:F:110:LEU:HD11	1:F:159:ARG:HD2	1.34	1.09
1:B:44:GLN:HG2	2:B:301:HOH:O	1.53	1.06
1:H:110:LEU:HD21	1:H:159:ARG:HE	1.25	1.02
1:D:62:VAL:HG13	1:D:78:LYS:NZ	1.76	0.98
1:D:110:LEU:HD11	1:D:159:ARG:HH12	1.29	0.97
1:G:110:LEU:HD11	1:G:159:ARG:HE	1.30	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:VAL:HG13	1:D:78:LYS:HZ1	1.25	0.96
1:B:8:VAL:H	1:B:110:LEU:HD23	1.31	0.95
1:A:7:ARG:HA	1:A:110:LEU:HD13	1.50	0.94
1:A:111:GLN:OE1	1:A:249:ALA:HB1	1.65	0.94
1:F:8:VAL:H	1:F:110:LEU:HD23	1.35	0.90
1:G:84:GLY:HA2	1:G:108:TYR:N	1.87	0.90
1:E:8:VAL:H	1:E:110:LEU:HD23	1.36	0.89
1:D:8:VAL:H	1:D:110:LEU:HD23	1.37	0.88
1:C:8:VAL:H	1:C:110:LEU:HD23	1.37	0.88
1:E:64:ALA:HB3	1:E:75:MET:CE	2.03	0.87
1:D:111:GLN:HE22	1:D:164:ILE:HD12	1.39	0.87
1:D:111:GLN:HE22	1:D:164:ILE:CD1	1.86	0.86
1:G:231:THR:HG21	2:G:370:HOH:O	1.75	0.86
1:H:7:ARG:HA	1:H:110:LEU:HD13	1.58	0.84
1:G:8:VAL:H	1:G:110:LEU:HD23	1.40	0.84
1:A:215:ARG:HD2	1:A:215:ARG:O	1.79	0.82
1:D:62:VAL:HG22	1:D:78:LYS:HE3	1.62	0.81
1:H:110:LEU:HD21	1:H:159:ARG:NE	1.95	0.81
1:A:111:GLN:HE22	1:A:162:ARG:HG3	1.44	0.80
1:B:110:LEU:HD11	1:B:159:ARG:HE	1.45	0.80
1:F:110:LEU:CD1	1:F:159:ARG:HD2	2.11	0.80
1:A:111:GLN:NE2	1:A:162:ARG:HB2	1.99	0.77
1:D:110:LEU:HD11	1:D:159:ARG:NH1	1.99	0.77
1:D:111:GLN:NE2	1:D:164:ILE:HD12	1.99	0.77
1:A:110:LEU:HD21	1:A:159:ARG:HD2	1.66	0.76
1:A:215:ARG:HD2	1:A:215:ARG:C	2.10	0.75
1:B:64:ALA:HB3	1:B:75:MET:HE2	1.69	0.74
1:D:111:GLN:OE1	1:D:249:ALA:CB	2.36	0.74
1:E:28:ASP:OD2	1:E:55:LYS:HE2	1.86	0.74
1:B:8:VAL:N	1:B:110:LEU:HD23	2.02	0.74
1:A:57:ARG:HD2	2:A:305:HOH:O	1.88	0.72
1:E:28:ASP:OD2	1:E:55:LYS:CE	2.38	0.72
1:E:36:ASN:ND2	1:E:75:MET:HE1	2.06	0.71
1:C:8:VAL:N	1:C:110:LEU:HD23	2.06	0.71
1:H:175:MET:HE3	1:H:178:LEU:CD1	2.20	0.71
1:B:60:LEU:HD22	1:B:62:VAL:HG13	1.73	0.71
1:F:111:GLN:CD	1:F:249:ALA:HB1	2.15	0.70
1:D:111:GLN:OE1	1:D:249:ALA:HB1	1.91	0.70
1:H:175:MET:HE3	1:H:178:LEU:HD12	1.73	0.70
1:A:111:GLN:HE21	1:A:162:ARG:HB2	1.57	0.69
1:F:8:VAL:N	1:F:110:LEU:HD23	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:GLY:HA2	1:D:108:TYR:N	2.09	0.67
2:E:392:HOH:O	1:F:129:LEU:HD12	1.94	0.67
1:F:84:GLY:HA3	1:F:108:TYR:N	2.12	0.65
1:G:158:GLY:HA2	2:G:378:HOH:O	1.96	0.65
1:E:8:VAL:N	1:E:110:LEU:HD23	2.10	0.64
1:C:84:GLY:CA	1:C:108:TYR:N	2.61	0.63
1:A:8:VAL:H	1:A:110:LEU:HD12	1.64	0.63
1:D:84:GLY:CA	1:D:108:TYR:N	2.62	0.62
1:G:8:VAL:N	1:G:110:LEU:HD23	2.13	0.61
1:H:172:LYS:HE2	1:H:270:ASP:OD1	2.02	0.60
1:E:110:LEU:HD11	1:E:159:ARG:HD2	1.84	0.60
1:D:8:VAL:N	1:D:110:LEU:HD23	2.12	0.60
1:G:110:LEU:HD11	1:G:159:ARG:NE	2.11	0.59
1:G:60:LEU:HD23	1:G:61:ALA:O	2.02	0.59
1:A:111:GLN:HE22	1:A:162:ARG:CG	2.16	0.59
1:B:124:LEU:HD21	1:C:147:TYR:HB3	1.86	0.58
1:F:110:LEU:HD11	1:F:159:ARG:CD	2.23	0.58
1:B:60:LEU:HD11	1:B:82:GLU:HG3	1.86	0.57
1:D:62:VAL:HG22	1:D:78:LYS:CE	2.34	0.57
1:G:60:LEU:HD22	1:G:62:VAL:HG13	1.85	0.57
1:F:172:LYS:HE3	1:F:270:ASP:OD2	2.05	0.57
1:C:84:GLY:HA3	1:C:108:TYR:N	2.20	0.56
1:H:110:LEU:HD22	2:H:333:HOH:O	2.05	0.56
1:H:199:PHE:HB3	1:H:204:ILE:HB	1.87	0.56
1:H:84:GLY:C	1:H:108:TYR:CB	2.78	0.56
1:D:215:ARG:HG2	1:D:238:PRO:HD3	1.87	0.56
1:A:111:GLN:NE2	1:A:162:ARG:CB	2.68	0.56
1:G:199:PHE:HB3	1:G:204:ILE:HB	1.87	0.56
1:A:18:LEU:HD12	1:A:238:PRO:HB3	1.89	0.55
1:E:36:ASN:ND2	1:E:75:MET:CE	2.70	0.55
1:A:111:GLN:NE2	1:A:162:ARG:HG3	2.19	0.55
1:H:8:VAL:H	1:H:110:LEU:HD12	1.72	0.55
1:H:31:LEU:HD21	1:H:111:GLN:HE21	1.70	0.54
1:A:111:GLN:NE2	1:A:162:ARG:CG	2.71	0.54
1:H:213:GLY:O	1:H:235:PHE:HA	2.08	0.54
1:A:176:ILE:HD11	1:D:198:GLU:HA	1.90	0.53
1:H:84:GLY:C	2:H:304:HOH:O	2.51	0.53
1:B:199:PHE:HB3	1:B:204:ILE:HB	1.90	0.53
1:F:7:ARG:HA	1:F:110:LEU:HD23	1.91	0.53
1:G:12:THR:O	1:G:115:ASN:HB3	2.09	0.53
1:G:31:LEU:HD21	1:G:111:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ALA:CB	1:E:75:MET:CE	2.84	0.52
1:G:84:GLY:CA	1:G:108:TYR:N	2.68	0.52
1:H:73:GLN:HG2	2:H:380:HOH:O	2.09	0.52
1:H:170:ALA:HB2	1:H:175:MET:HE2	1.91	0.52
1:H:111:GLN:OE1	1:H:249:ALA:HB1	2.10	0.52
1:A:147:TYR:HB3	1:D:124:LEU:HD21	1.90	0.52
1:B:64:ALA:HB1	1:B:71:ASP:HB3	1.92	0.52
1:D:119:VAL:HG12	1:D:181:TYR:CE1	2.45	0.52
1:A:12:THR:O	1:A:115:ASN:HB3	2.09	0.52
1:D:41:LYS:NZ	2:D:302:HOH:O	2.44	0.52
1:F:237:ASP:CG	1:F:238:PRO:HD2	2.35	0.51
1:A:7:ARG:HA	1:A:110:LEU:CD1	2.33	0.51
1:E:233:LEU:HD21	2:E:459:HOH:O	2.10	0.51
1:G:7:ARG:HA	1:G:110:LEU:HD23	1.93	0.51
1:B:213:GLY:O	1:B:235:PHE:HA	2.11	0.51
1:D:62:VAL:HG13	1:D:78:LYS:CE	2.39	0.51
1:D:111:GLN:NE2	1:D:164:ILE:CD1	2.64	0.51
1:C:31:LEU:O	1:C:57:ARG:HD3	2.11	0.51
1:C:42:SER:O	1:C:46:GLN:NE2	2.43	0.51
1:F:237:ASP:OD2	1:F:238:PRO:HD2	2.10	0.51
1:B:119:VAL:O	1:B:120:LEU:HD23	2.11	0.50
1:G:173:LYS:O	1:G:175:MET:HE2	2.10	0.50
1:C:235:PHE:CD2	1:C:235:PHE:C	2.90	0.50
1:E:124:LEU:HD21	1:F:147:TYR:HB3	1.92	0.50
1:B:129:LEU:H	1:B:129:LEU:HD22	1.75	0.50
1:D:199:PHE:HB3	1:D:204:ILE:HB	1.94	0.50
1:E:237:ASP:CG	1:E:238:PRO:HD2	2.37	0.50
1:F:199:PHE:HB3	1:F:204:ILE:HB	1.93	0.50
1:G:231:THR:CG2	1:G:233:LEU:H	2.25	0.50
1:A:69:ASP:HB2	1:D:129:LEU:HD21	1.94	0.49
1:D:62:VAL:HG11	1:D:75:MET:HG3	1.95	0.48
1:G:147:TYR:HB3	1:H:124:LEU:HD21	1.94	0.48
1:F:270:ASP:OD1	1:G:270:ASP:CB	2.61	0.48
1:F:26:LEU:HD22	1:F:111:GLN:HE22	1.77	0.48
1:G:60:LEU:CD2	1:G:62:VAL:HG13	2.44	0.48
1:G:64:ALA:HB1	1:G:71:ASP:HB3	1.95	0.48
1:C:12:THR:O	1:C:115:ASN:HB3	2.13	0.48
1:A:111:GLN:CD	1:A:249:ALA:HB1	2.37	0.47
1:B:187:ALA:HB2	1:C:187:ALA:HB2	1.95	0.47
1:G:83:LEU:O	1:G:84:GLY:C	2.58	0.47
1:C:244:LEU:HD22	1:C:263:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:LYS:HB3	1:D:78:LYS:HE2	1.64	0.47
1:H:110:LEU:HD21	1:H:159:ARG:CD	2.45	0.47
1:H:164:ILE:HA	1:H:207:ASN:O	2.15	0.47
1:E:199:PHE:HB3	1:E:204:ILE:HB	1.96	0.46
1:E:64:ALA:HB3	1:E:75:MET:HE3	1.93	0.46
1:H:8:VAL:H	1:H:110:LEU:CD1	2.27	0.46
1:B:66:VAL:HG12	1:B:142:GLY:CA	2.46	0.46
1:C:213:GLY:O	1:C:235:PHE:HA	2.16	0.46
1:G:36:ASN:ND2	1:G:75:MET:HE2	2.31	0.46
1:H:168:SER:HB3	1:H:185:LYS:HG3	1.97	0.46
1:A:7:ARG:CA	1:A:110:LEU:HD13	2.34	0.46
1:F:163:ILE:O	1:F:206:VAL:HA	2.16	0.46
1:H:172:LYS:HE2	1:H:270:ASP:CG	2.41	0.46
1:B:18:LEU:HD12	1:B:238:PRO:HB3	1.96	0.46
1:G:213:GLY:O	1:G:235:PHE:HA	2.15	0.46
1:H:110:LEU:C	1:H:111:GLN:HG2	2.40	0.46
1:H:12:THR:O	1:H:115:ASN:HB3	2.15	0.45
1:H:9:ALA:HA	1:H:111:GLN:O	2.17	0.45
1:A:199:PHE:HB3	1:A:204:ILE:HB	1.99	0.45
1:E:64:ALA:HB3	1:E:75:MET:HE1	1.94	0.45
1:A:8:VAL:H	1:A:110:LEU:CD1	2.27	0.45
1:C:199:PHE:HB3	1:C:204:ILE:HB	1.99	0.45
1:A:213:GLY:O	1:A:235:PHE:HA	2.17	0.44
1:B:9:ALA:HA	1:B:111:GLN:O	2.17	0.44
1:B:12:THR:O	1:B:115:ASN:HB3	2.16	0.44
1:H:111:GLN:CD	1:H:249:ALA:HB1	2.42	0.44
1:H:148:LYS:O	1:H:152:VAL:HG23	2.17	0.44
1:B:60:LEU:CD1	1:B:82:GLU:HB2	2.48	0.44
1:B:178:LEU:N	1:B:179:PRO:CD	2.80	0.44
1:E:28:ASP:OD2	1:E:55:LYS:HE3	2.16	0.44
1:A:215:ARG:C	1:A:215:ARG:CD	2.85	0.44
1:G:18:LEU:HD21	1:G:241:VAL:HG21	1.98	0.44
1:H:172:LYS:NZ	1:H:270:ASP:OD2	2.51	0.44
1:A:141:ARG:NH1	1:D:133:ASP:OD1	2.51	0.44
1:B:66:VAL:HG12	1:B:142:GLY:HA2	2.00	0.44
1:C:163:ILE:O	1:C:206:VAL:HA	2.18	0.44
1:G:31:LEU:CD2	1:G:111:GLN:CD	2.91	0.44
1:F:148:LYS:NZ	2:F:307:HOH:O	2.51	0.43
1:A:124:LEU:HD12	1:A:124:LEU:HA	1.90	0.43
1:B:163:ILE:O	1:B:206:VAL:HA	2.19	0.43
1:G:26:LEU:HD22	1:G:111:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:N	1:C:179:PRO:CD	2.81	0.43
1:A:9:ALA:HA	1:A:111:GLN:O	2.19	0.43
1:C:132:TRP:CE3	1:C:180:ALA:HB2	2.54	0.43
1:D:116:ALA:O	2:D:301:HOH:O	2.21	0.43
1:F:258:GLY:HA3	1:G:269:PHE:CE1	2.54	0.43
1:E:33:VAL:HB	1:E:52:ILE:HD13	2.01	0.43
1:A:124:LEU:HD21	1:D:147:TYR:HB3	2.00	0.42
1:A:176:ILE:CD1	1:D:198:GLU:HA	2.49	0.42
1:E:158:GLY:HA2	2:E:386:HOH:O	2.19	0.42
1:G:124:LEU:HD12	1:G:124:LEU:HA	1.89	0.42
1:E:36:ASN:HD22	1:E:75:MET:CE	2.31	0.42
1:G:31:LEU:HD21	1:G:111:GLN:CD	2.44	0.42
1:H:133:ASP:OD2	2:H:301:HOH:O	2.21	0.42
1:A:33:VAL:O	1:A:59:ALA:HA	2.19	0.42
1:G:231:THR:HG23	1:G:233:LEU:H	1.83	0.42
1:F:164:ILE:HA	1:F:207:ASN:O	2.20	0.42
1:G:111:GLN:CD	1:G:249:ALA:HB1	2.45	0.42
1:A:163:ILE:O	1:A:206:VAL:HA	2.20	0.42
1:F:108:TYR:CB	1:F:159:ARG:HH12	2.32	0.42
1:G:14:ALA:HA	1:G:19:GLY:HA3	2.02	0.42
1:H:48:ILE:O	1:H:52:ILE:HG12	2.19	0.42
1:A:109:ASP:N	1:A:157:GLN:HE22	2.18	0.42
1:A:120:LEU:HB2	1:A:135:ILE:HD11	2.01	0.41
1:B:119:VAL:HG22	1:B:181:TYR:CE1	2.55	0.41
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.93	0.41
1:E:57:ARG:NE	2:E:308:HOH:O	2.50	0.41
1:B:111:GLN:O	1:B:111:GLN:HG3	2.17	0.41
1:H:64:ALA:HB1	1:H:71:ASP:HB3	2.02	0.41
1:F:165:ALA:O	1:F:208:ALA:HA	2.20	0.41
1:B:7:ARG:HA	1:B:110:LEU:HD23	2.01	0.41
1:C:200:ALA:N	1:C:201:PRO:CD	2.83	0.41
1:H:37:ASP:HB2	1:H:45:LEU:HD11	2.03	0.41
1:C:120:LEU:HB2	1:C:135:ILE:HD11	2.03	0.41
1:C:7:ARG:HA	1:C:110:LEU:HD23	2.02	0.41
1:C:233:LEU:HD12	1:C:233:LEU:N	2.36	0.41
1:H:7:ARG:CA	1:H:110:LEU:HD13	2.42	0.41
1:E:64:ALA:CB	1:E:75:MET:HE3	2.51	0.41
1:B:33:VAL:O	1:B:59:ALA:HA	2.22	0.40
1:E:64:ALA:HB3	1:E:75:MET:HE2	1.94	0.40
1:F:7:ARG:HD3	2:F:339:HOH:O	2.20	0.40
1:F:12:THR:O	1:F:115:ASN:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:O	1:D:59:ALA:HA	2.21	0.40
1:E:39:GLY:O	1:E:42:SER:HB2	2.22	0.40
1:E:120:LEU:HB2	1:E:135:ILE:HD11	2.02	0.40
1:B:200:ALA:HB3	1:B:201:PRO:HD3	2.03	0.40
1:G:129:LEU:HD12	1:G:129:LEU:HA	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/270 (82%)	214 (97%)	6 (3%)	0	100	100
1	B	221/270 (82%)	215 (97%)	6 (3%)	0	100	100
1	C	222/270 (82%)	216 (97%)	5 (2%)	1 (0%)	24	21
1	D	221/270 (82%)	215 (97%)	6 (3%)	0	100	100
1	E	221/270 (82%)	216 (98%)	5 (2%)	0	100	100
1	F	221/270 (82%)	216 (98%)	5 (2%)	0	100	100
1	G	226/270 (84%)	220 (97%)	6 (3%)	0	100	100
1	H	221/270 (82%)	217 (98%)	4 (2%)	0	100	100
All	All	1773/2160 (82%)	1729 (98%)	43 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	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	171/211 (81%)	166 (97%)	5 (3%)	37	40
1	B	172/211 (82%)	165 (96%)	7 (4%)	27	26
1	C	170/211 (81%)	166 (98%)	4 (2%)	43	47
1	D	172/211 (82%)	167 (97%)	5 (3%)	37	40
1	E	172/211 (82%)	166 (96%)	6 (4%)	32	32
1	F	172/211 (82%)	169 (98%)	3 (2%)	53	60
1	G	175/211 (83%)	170 (97%)	5 (3%)	37	40
1	H	170/211 (81%)	163 (96%)	7 (4%)	27	26
All	All	1374/1688 (81%)	1332 (97%)	42 (3%)	35	37

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	18	LEU
1	A	36	ASN
1	A	111	GLN
1	A	215	ARG
1	B	4	THR
1	B	47	GLN
1	B	111	GLN
1	B	127	THR
1	B	156	LYS
1	B	232	ASN
1	B	233	LEU
1	C	18	LEU
1	C	60	LEU
1	C	175	MET
1	C	270	ASP
1	D	5	SER
1	D	16	GLN
1	D	44	GLN

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Mol	Chain	Res	Type
1	D	78	LYS
1	D	111	GLN
1	E	18	LEU
1	E	28	ASP
1	E	36	ASN
1	E	127	THR
1	E	130	GLU
1	E	263	VAL
1	F	127	THR
1	F	215	ARG
1	F	270	ASP
1	G	62	VAL
1	G	127	THR
1	G	134	ARG
1	G	228	ASP
1	G	231	THR
1	H	45	LEU
1	H	119	VAL
1	H	127	THR
1	H	128	GLN
1	H	232	ASN
1	H	237	ASP
1	H	246	SER

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

Mol	Chain	Res	Type
1	A	46	GLN
1	A	51	GLN
1	A	111	GLN
1	B	51	GLN
1	B	115	ASN
1	C	16	GLN
1	D	44	GLN
1	D	46	GLN
1	D	47	GLN
1	D	177	ASN
1	D	202	HIS
1	E	153	GLN
1	E	157	GLN
1	F	47	GLN
1	F	111	GLN

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Mol	Chain	Res	Type
1	F	177	ASN
1	G	36	ASN
1	G	111	GLN
1	G	203	ASN
1	H	115	ASN
1	H	122	GLN
1	H	177	ASN

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	226/270 (83%)	-0.44	3 (1%) 75 74	11, 18, 32, 55	0
1	B	227/270 (84%)	-0.47	5 (2%) 62 61	12, 18, 34, 60	0
1	C	228/270 (84%)	-0.42	6 (2%) 57 56	11, 18, 31, 65	0
1	D	227/270 (84%)	-0.37	4 (1%) 67 67	12, 19, 31, 50	0
1	E	227/270 (84%)	-0.39	2 (0%) 81 80	13, 19, 34, 59	0
1	F	227/270 (84%)	-0.33	4 (1%) 67 67	13, 20, 33, 57	0
1	G	232/270 (85%)	-0.30	5 (2%) 62 61	12, 20, 39, 52	0
1	H	227/270 (84%)	-0.33	5 (2%) 62 61	12, 21, 40, 52	0
All	All	1821/2160 (84%)	-0.38	34 (1%) 66 66	11, 19, 35, 65	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	GLY	5.4
1	G	84	GLY	5.4
1	C	84	GLY	5.3
1	H	270	ASP	4.5
1	G	111	GLN	4.2
1	F	111	GLN	4.0
1	B	111	GLN	3.5
1	A	111	GLN	3.3
1	H	84	GLY	3.1
1	F	84	GLY	3.1
1	F	270	ASP	3.1
1	G	226	LEU	3.0
1	D	111	GLN	3.0
1	C	232	ASN	2.9
1	C	239	GLU	2.7
1	G	228	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	235	PHE	2.7
1	H	111	GLN	2.7
1	G	232	ASN	2.6
1	E	270	ASP	2.6
1	B	235	PHE	2.5
1	B	108	TYR	2.4
1	C	108	TYR	2.4
1	B	4	THR	2.3
1	C	216	THR	2.3
1	B	232	ASN	2.3
1	H	108	TYR	2.2
1	D	108	TYR	2.2
1	C	270	ASP	2.1
1	A	215	ARG	2.1
1	A	270	ASP	2.1
1	D	270	ASP	2.1
1	F	237	ASP	2.1
1	H	215	ARG	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.