



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:51 AM UTC

PDB ID : 8OJ9 / pdb_00008oj9
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 free form
Authors : Haesaerts, S.; Loris, R.; Larsen, P.B.
Deposited on : 2023-03-24
Resolution : 3.25 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

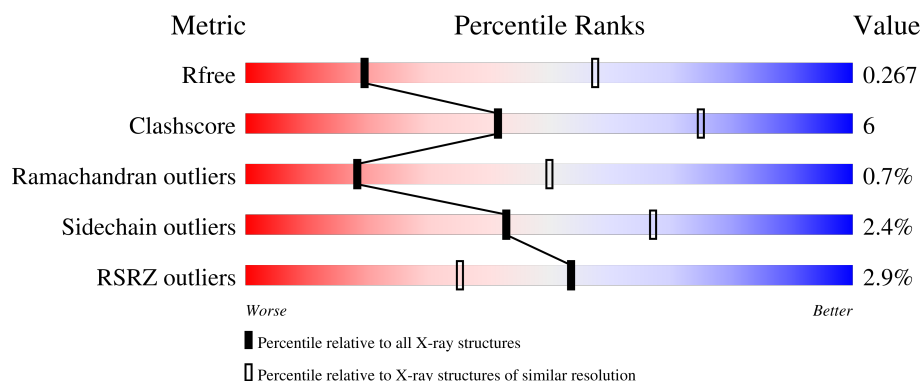
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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 $\leq 5\%$. 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	974	 3% 82% 15% ..
1	B	974	 3% 80% 16% ..
1	C	974	 2% 76% 20% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22790 atoms, of which 0 are hydrogens and 0 are deuteriums.

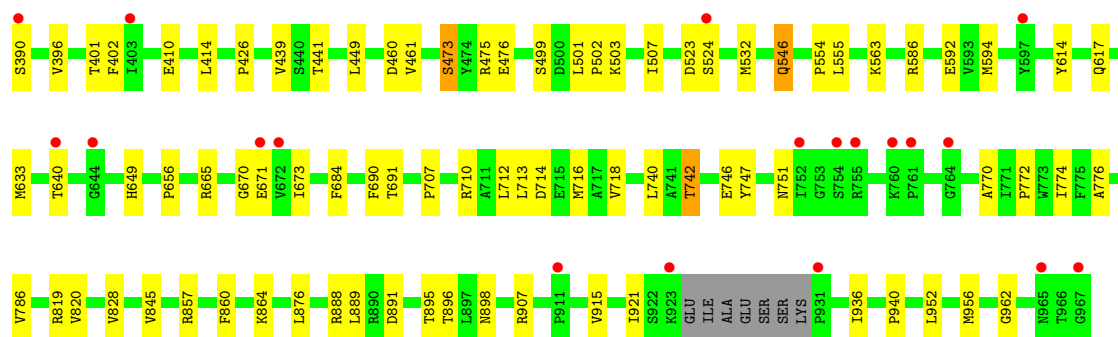
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphoenolpyruvate carboxylase 1.

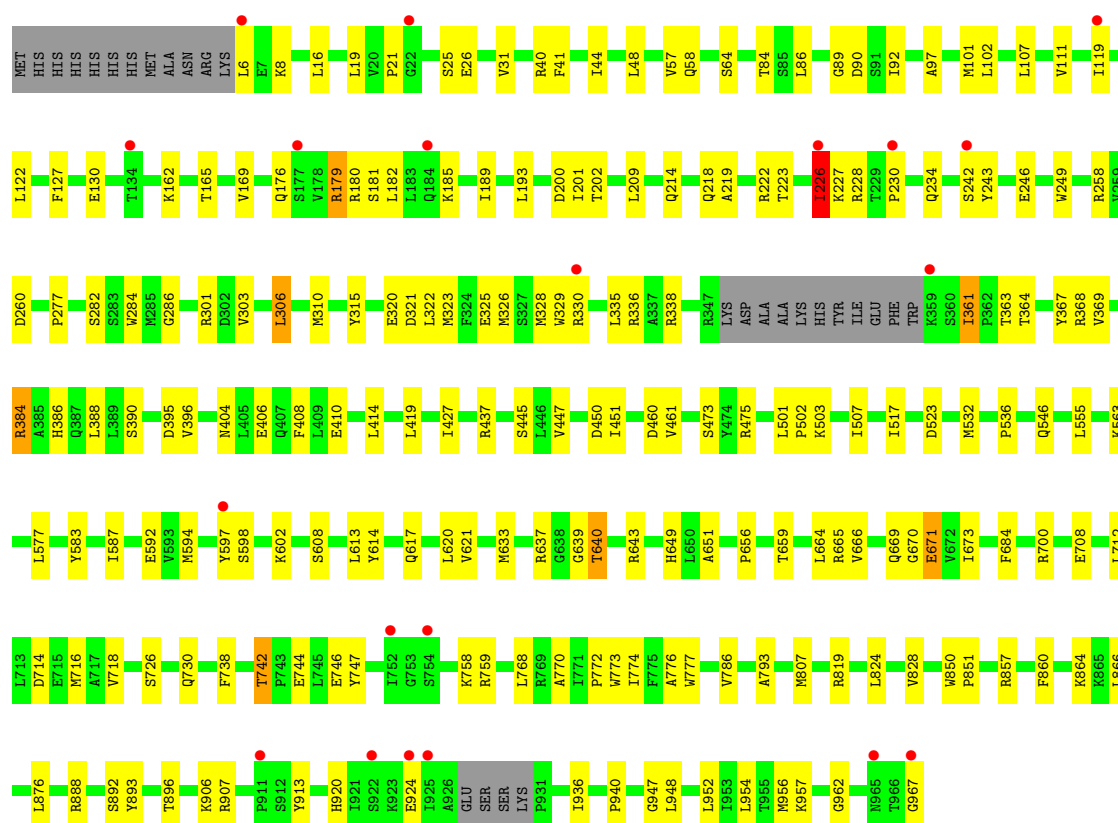
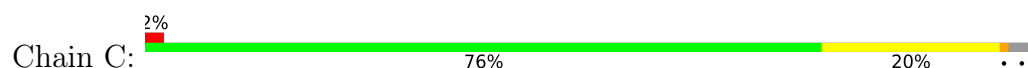
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	944	Total	C	N	O	S	0	3	1
			7587	4807	1326	1424	30			
1	B	943	Total	C	N	O	S	0	3	0
			7586	4807	1325	1424	30			
1	C	947	Total	C	N	O	S	0	4	1
			7617	4826	1332	1429	30			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9MAH0
A	-5	HIS	-	expression tag	UNP Q9MAH0
A	-4	HIS	-	expression tag	UNP Q9MAH0
A	-3	HIS	-	expression tag	UNP Q9MAH0
A	-2	HIS	-	expression tag	UNP Q9MAH0
A	-1	HIS	-	expression tag	UNP Q9MAH0
A	0	HIS	-	expression tag	UNP Q9MAH0
B	-6	MET	-	initiating methionine	UNP Q9MAH0
B	-5	HIS	-	expression tag	UNP Q9MAH0
B	-4	HIS	-	expression tag	UNP Q9MAH0
B	-3	HIS	-	expression tag	UNP Q9MAH0
B	-2	HIS	-	expression tag	UNP Q9MAH0
B	-1	HIS	-	expression tag	UNP Q9MAH0
B	0	HIS	-	expression tag	UNP Q9MAH0
C	-6	MET	-	initiating methionine	UNP Q9MAH0
C	-5	HIS	-	expression tag	UNP Q9MAH0
C	-4	HIS	-	expression tag	UNP Q9MAH0
C	-3	HIS	-	expression tag	UNP Q9MAH0
C	-2	HIS	-	expression tag	UNP Q9MAH0
C	-1	HIS	-	expression tag	UNP Q9MAH0
C	0	HIS	-	expression tag	UNP Q9MAH0



● Molecule 1: Phosphoenolpyruvate carboxylase 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	244.35Å 244.35Å 397.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 3.25 48.50 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.50-3.25) 99.6 (48.50-3.25)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.228 , 0.264 0.233 , 0.267	Depositor DCC
R_{free} test set	4677 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 105.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22790	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2326e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.24	0/7756	0.44	0/10495
1	B	0.23	0/7755	0.45	0/10493
1	C	0.30	0/7789	0.50	0/10539
All	All	0.26	0/23300	0.46	0/31527

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7587	0	7573	87	0
1	B	7586	0	7573	100	0
1	C	7617	0	7608	112	1
All	All	22790	0	22754	289	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 6.

All (289) 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:C:119:ILE:HD12	1:C:122:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HB2	1:B:921:ILE:HG21	1.64	0.77
1:A:119:ILE:HD12	1:A:122:LEU:HD22	1.68	0.75
1:B:952:LEU:HG	1:B:956:MET:HE2	1.70	0.73
1:A:301:ARG:NH2	1:A:388:LEU:O	2.22	0.73
1:C:952:LEU:HG	1:C:956:MET:HE2	1.72	0.72
1:C:301:ARG:NH2	1:C:388:LEU:O	2.23	0.72
1:A:169:VAL:HG22	1:A:282:SER:HB2	1.75	0.69
1:C:786:VAL:HG11	1:C:828:VAL:HG21	1.75	0.69
1:A:617:GLN:HG2	1:A:633:MET:HE2	1.76	0.68
1:A:460:ASP:OD1	1:A:475:ARG:NH2	2.26	0.67
1:C:460:ASP:OD1	1:C:475:ARG:NH2	2.28	0.67
1:C:328:MET:HE2	1:C:427:ILE:HD13	1.76	0.66
1:A:786:VAL:HG11	1:A:828:VAL:HG21	1.77	0.66
1:C:335:LEU:HD12	1:C:414:LEU:HG	1.78	0.66
1:C:361:ILE:HG21	1:C:369:VAL:HA	1.78	0.65
1:A:84:THR:O	1:A:907:ARG:NH2	2.30	0.64
1:A:857:ARG:O	1:A:860:PHE:HB3	1.97	0.63
1:B:857:ARG:O	1:B:860:PHE:HB3	1.99	0.63
1:B:286:GLY:HA3	1:B:303:VAL:HG21	1.82	0.62
1:A:532:MET:CG	1:A:759:ARG:HH12	2.11	0.62
1:B:40:ARG:HD2	1:B:214:GLN:HG2	1.82	0.62
1:C:169:VAL:HG22	1:C:282:SER:HB2	1.82	0.62
1:C:461:VAL:HG22	1:C:507:ILE:HG23	1.80	0.61
1:C:857:ARG:O	1:C:860:PHE:HB3	2.01	0.61
1:B:44:ILE:HD13	1:B:218:GLN:HB2	1.83	0.61
1:C:451:ILE:HG13	1:C:517:ILE:HD11	1.82	0.60
1:A:48:LEU:HD22	1:A:222:ARG:NH1	2.17	0.59
1:C:864:LYS:HE2	1:C:876:LEU:HD11	1.84	0.59
1:C:336:ARG:NH1	1:C:363:THR:O	2.34	0.59
1:A:102:LEU:HD21	1:A:962:GLY:HA3	1.85	0.59
1:B:102:LEU:HD21	1:B:962:GLY:HA3	1.83	0.59
1:C:323:MET:O	1:C:368:ARG:NH1	2.35	0.58
1:B:53:LEU:HD23	1:B:921:ILE:HG13	1.86	0.58
1:A:362:PRO:HB2	1:B:228:ARG:HH21	1.67	0.57
1:C:8:LYS:HB3	1:C:58:GLN:HE22	1.69	0.57
1:C:338:ARG:NH2	1:C:410:GLU:OE1	2.28	0.57
1:A:643:ARG:HD2	1:A:824:LEU:HD12	1.85	0.56
1:A:746:GLU:OE2	1:A:746:GLU:N	2.36	0.56
1:B:712:LEU:O	1:B:716:MET:HG3	2.06	0.56
1:A:637[B]:ARG:HG3	1:A:669:GLN:HG2	1.88	0.56
1:C:546:GLN:OE1	1:C:555:LEU:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:LYS:HE2	1:A:876:LEU:HD11	1.88	0.55
1:C:286:GLY:HA3	1:C:303:VAL:HG21	1.88	0.55
1:A:8:LYS:HB3	1:A:58:GLN:HE22	1.71	0.55
1:C:179:ARG:HH12	1:C:181:SER:HB3	1.71	0.55
1:A:258:ARG:HG2	1:A:684:PHE:HZ	1.69	0.55
1:C:384:ARG:HG2	1:C:396:VAL:HB	1.88	0.55
1:B:258:ARG:HG2	1:B:684:PHE:HZ	1.72	0.54
1:A:179:ARG:HH12	1:A:181:SER:HB3	1.73	0.54
1:B:130:GLU:OE2	1:B:145:LYS:NZ	2.40	0.54
1:B:746:GLU:OE2	1:B:746:GLU:N	2.33	0.54
1:B:338:ARG:NH2	1:B:410:GLU:OE1	2.28	0.54
1:C:41:PHE:HE2	1:C:101:MET:HE2	1.72	0.54
1:B:243:TYR:HA	1:B:246:GLU:HB2	1.90	0.54
1:A:598:SER:OG	1:A:967:GLY:OXT	2.26	0.53
1:B:532:MET:HE1	1:B:563:LYS:HD2	1.89	0.53
1:B:864:LYS:HE2	1:B:876:LEU:HD11	1.89	0.53
1:A:404:ASN:ND2	1:A:406:GLU:HB2	2.24	0.53
1:C:742:THR:HG22	1:C:744:GLU:H	1.74	0.53
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.91	0.53
1:C:258:ARG:HG2	1:C:684:PHE:HZ	1.73	0.53
1:C:179:ARG:NH1	1:C:181:SER:HB3	2.24	0.52
1:B:328:MET:SD	1:B:328:MET:N	2.81	0.52
1:C:532:MET:CG	1:C:759:ARG:HH12	2.21	0.52
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.91	0.52
1:A:284:TRP:CD1	1:A:450:ASP:HB2	2.44	0.52
1:A:532:MET:HG3	1:A:759:ARG:HH12	1.75	0.52
1:B:449:LEU:N	1:B:524:SER:O	2.30	0.52
1:C:536:PRO:HB3	1:C:577:LEU:HG	1.92	0.52
1:C:742:THR:HG21	1:C:776:ALA:HB1	1.92	0.52
1:B:384:ARG:HD2	1:B:401:THR:HG21	1.92	0.52
1:B:48:LEU:HD22	1:B:222:ARG:NH1	2.26	0.51
1:C:57:VAL:CG1	1:C:101:MET:HE1	2.40	0.51
1:C:617:GLN:HG2	1:C:633:MET:HE2	1.91	0.51
1:B:252:VAL:HG21	1:B:441:THR:HG21	1.92	0.51
1:A:48:LEU:HD13	1:A:222:ARG:HD3	1.92	0.51
1:C:16:LEU:HB3	1:C:31:VAL:HG13	1.92	0.51
1:B:57:VAL:CG1	1:B:101:MET:HE1	2.40	0.51
1:A:332:ASN:HB2	1:A:418:SER:HA	1.93	0.51
1:B:16:LEU:HB3	1:B:31:VAL:HG13	1.93	0.51
1:B:84:THR:O	1:B:907:ARG:NH2	2.44	0.51
1:B:336:ARG:NH1	1:B:363:THR:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:TYR:O	1:C:587:ILE:HG23	2.11	0.50
1:A:536:PRO:HB3	1:A:577:LEU:HG	1.92	0.50
1:B:301:ARG:NH2	1:B:388:LEU:O	2.44	0.50
1:B:41:PHE:HE1	1:B:101:MET:HE2	1.76	0.50
1:C:127:PHE:HE2	1:C:819:ARG:HD2	1.76	0.50
1:C:742:THR:CG2	1:C:776:ALA:HB1	2.42	0.50
1:B:460:ASP:OD1	1:B:475:ARG:NH2	2.44	0.50
1:B:41:PHE:CE1	1:B:101:MET:HE2	2.46	0.50
1:A:532:MET:HE1	1:A:563:LYS:HD2	1.93	0.50
1:C:234:GLN:OE1	1:C:234:GLN:N	2.38	0.50
1:B:182:LEU:HD12	1:B:185:LYS:HD2	1.94	0.49
1:C:102:LEU:HD21	1:C:962:GLY:HA3	1.94	0.49
1:C:598:SER:OG	1:C:967:GLY:OXT	2.29	0.49
1:A:328:MET:HE2	1:A:427:ILE:HD13	1.95	0.49
1:B:384:ARG:HG3	1:B:396:VAL:HB	1.94	0.49
1:C:592:GLU:OE2	1:C:665:ARG:NH1	2.45	0.49
1:B:501:LEU:O	1:B:503:LYS:HG3	2.13	0.49
1:B:592:GLU:OE2	1:B:665:ARG:NH1	2.46	0.49
1:C:226:ILE:HD12	1:C:227:LYS:HG3	1.95	0.49
1:C:249:TRP:HH2	1:C:315:TYR:CD1	2.31	0.49
1:C:284:TRP:CD1	1:C:450:ASP:HB2	2.47	0.49
1:C:243:TYR:HA	1:C:246:GLU:HB2	1.95	0.49
1:B:323:MET:O	1:B:368:ARG:NH1	2.41	0.48
1:A:712:LEU:O	1:A:716:MET:HG3	2.13	0.48
1:C:41:PHE:CE2	1:C:101:MET:HE2	2.48	0.48
1:B:499:SER:O	1:B:503:LYS:NZ	2.45	0.48
1:A:284:TRP:CH2	1:A:594:MET:HE1	2.48	0.48
1:A:285:MET:HE3	1:A:285:MET:HB2	1.73	0.48
1:C:716:MET:HB3	1:C:793:ALA:HB1	1.95	0.48
1:B:237:MET:O	1:B:241:MET:HG2	2.13	0.48
1:C:501:LEU:O	1:C:503:LYS:HG3	2.14	0.48
1:A:127:PHE:HE1	1:A:819:ARG:HD2	1.79	0.48
1:A:364:THR:HG23	1:B:228:ARG:HH22	1.77	0.48
1:C:44:ILE:HD13	1:C:218:GLN:HB2	1.95	0.48
1:A:330:ARG:HD3	1:B:222:ARG:CZ	2.43	0.48
1:B:185:LYS:O	1:B:189:ILE:HG13	2.14	0.48
1:C:747:TYR:HE2	1:C:772:PRO:HG3	1.79	0.48
1:A:215:ARG:HD3	1:B:426:PRO:O	2.13	0.48
1:A:501:LEU:HD12	1:A:502:PRO:HD2	1.95	0.48
1:B:377:LYS:HD2	1:B:402:PHE:CE1	2.49	0.48
1:C:306:LEU:O	1:C:310:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLU:HB3	1:B:375:ARG:HH12	1.79	0.47
1:B:501:LEU:HB3	1:B:503:LYS:HE3	1.96	0.47
1:C:532:MET:HG3	1:C:759:ARG:HH12	1.79	0.47
1:C:712:LEU:O	1:C:716:MET:HG3	2.14	0.47
1:A:670:GLY:O	1:A:673:ILE:HG22	2.14	0.47
1:C:97:ALA:C	1:C:101:MET:HE3	2.39	0.47
1:A:286:GLY:HA3	1:A:303:VAL:HG21	1.96	0.47
1:A:362:PRO:HB2	1:B:228:ARG:NH2	2.29	0.47
1:C:8:LYS:H	1:C:8:LYS:HG2	1.54	0.47
1:C:40:ARG:HD2	1:C:214:GLN:HG2	1.95	0.47
1:A:320:GLU:HB3	1:A:375:ARG:HH12	1.80	0.47
1:B:617:GLN:HG2	1:B:633:MET:HE2	1.96	0.47
1:C:284:TRP:CH2	1:C:594:MET:HE1	2.50	0.47
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.97	0.47
1:B:747:TYR:HE2	1:B:772:PRO:HG3	1.80	0.47
1:A:46:GLN:OE1	1:A:54:ARG:NH1	2.46	0.46
1:A:952:LEU:HG	1:A:956:MET:HE2	1.97	0.46
1:A:67:TYR:OH	1:A:833:ASP:OD2	2.26	0.46
1:B:97:ALA:C	1:B:101:MET:HE3	2.40	0.46
1:A:86:LEU:HB3	1:A:90:ASP:HB2	1.96	0.46
1:A:315:TYR:OH	1:A:439:VAL:HA	2.14	0.46
1:A:451:ILE:HG13	1:A:517:ILE:HD11	1.97	0.46
1:A:740:LEU:HD13	1:A:845:VAL:HA	1.97	0.46
1:B:57:VAL:HG11	1:B:101:MET:HE1	1.96	0.46
1:B:309:MET:HE2	1:B:309:MET:HB3	1.88	0.46
1:C:758:LYS:HG2	1:C:768:LEU:HA	1.98	0.46
1:B:64:SER:OG	1:B:896:THR:OG1	2.13	0.46
1:C:57:VAL:HG13	1:C:101:MET:HE1	1.98	0.46
1:C:325:GLU:HG3	1:C:326:MET:HE2	1.97	0.46
1:A:249:TRP:HH2	1:A:315:TYR:CD1	2.34	0.46
1:A:532:MET:HG2	1:A:759:ARG:HH12	1.80	0.46
1:B:169:VAL:HG22	1:B:282:SER:HB2	1.97	0.46
1:A:426:PRO:O	1:B:215:ARG:HD3	2.16	0.45
1:A:614:TYR:CD2	1:A:656:PRO:HG3	2.52	0.45
1:B:770:ALA:O	1:B:774:ILE:HG12	2.16	0.45
1:A:500:ASP:OD1	1:A:500:ASP:N	2.48	0.45
1:B:707:PRO:HA	1:B:710:ARG:HG3	1.97	0.45
1:C:637[B]:ARG:HG3	1:C:669:GLN:HG2	1.99	0.45
1:C:670:GLY:O	1:C:673:ILE:HG22	2.16	0.45
1:A:101:MET:HB3	1:A:893:TYR:CE1	2.52	0.45
1:A:874:LYS:HA	1:A:874:LYS:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PHE:HE2	1:B:819:ARG:HD2	1.81	0.45
1:B:166:VAL:HG11	1:B:690:PHE:HB3	1.99	0.45
1:A:742:THR:CG2	1:A:776:ALA:HB1	2.45	0.45
1:C:315:TYR:CE2	1:C:408:PHE:HE2	2.34	0.45
1:A:335:LEU:HD12	1:A:414:LEU:HG	1.98	0.45
1:A:770:ALA:O	1:A:774:ILE:HG12	2.17	0.45
1:C:180:ARG:HD2	1:C:242:SER:OG	2.16	0.45
1:C:329:TRP:CZ3	1:C:330:ARG:HG3	2.51	0.45
1:C:738:PHE:HD1	1:C:777:TRP:CZ2	2.34	0.45
1:A:260:ASP:CG	1:A:437:ARG:HH22	2.24	0.45
1:B:335:LEU:HD12	1:B:414:LEU:HG	1.99	0.45
1:C:19:LEU:HD21	1:C:892:SER:HB3	1.99	0.45
1:A:430:GLY:HA3	1:B:215:ARG:HD2	2.00	0.44
1:B:554:PRO:HG2	1:B:586:ARG:NH1	2.32	0.44
1:C:532:MET:HE1	1:C:563:LYS:HD2	1.99	0.44
1:A:583:TYR:O	1:A:587:ILE:HG23	2.17	0.44
1:C:176:GLN:CD	1:C:957:LYS:HD3	2.42	0.44
1:C:404:ASN:ND2	1:C:406:GLU:HB2	2.32	0.44
1:C:445:SER:O	1:C:447:VAL:N	2.45	0.44
1:C:850:TRP:N	1:C:851:PRO:HD2	2.32	0.44
1:B:230:PRO:HG3	1:B:751:ASN:HB3	2.00	0.44
1:B:546:GLN:OE1	1:B:555:LEU:N	2.45	0.44
1:A:411:PRO:O	1:A:414:LEU:HB3	2.18	0.44
1:A:501:LEU:O	1:A:503:LYS:HG3	2.17	0.44
1:B:201:ILE:HD12	1:B:201:ILE:HA	1.78	0.44
1:C:89:GLY:HA3	1:C:920:HIS:HE1	1.83	0.44
1:B:97:ALA:HB1	1:B:101:MET:CE	2.47	0.44
1:B:501:LEU:HD12	1:B:502:PRO:HD2	2.00	0.44
1:C:643:ARG:HD2	1:C:824:LEU:HD12	2.00	0.44
1:C:597[B]:TYR:CD2	1:C:639:GLY:HA2	2.53	0.44
1:A:816:PRO:O	1:A:820:VAL:HG13	2.17	0.44
1:B:179:ARG:HH12	1:B:181:SER:HB3	1.82	0.44
1:B:670:GLY:O	1:B:673:ILE:HG22	2.18	0.44
1:C:92:ILE:HD11	1:C:947:GLY:HA2	2.00	0.43
1:C:866:LEU:HD23	1:C:866:LEU:HA	1.85	0.43
1:A:364:THR:H	1:B:228:ARG:NH2	2.16	0.43
1:A:742:THR:HG21	1:A:776:ALA:HB1	2.00	0.43
1:B:130:GLU:O	1:B:649:HIS:HB3	2.19	0.43
1:B:742:THR:CG2	1:B:776:ALA:HB1	2.49	0.43
1:C:86:LEU:HB3	1:C:90:ASP:HB2	1.98	0.43
1:C:219:ALA:O	1:C:223:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:LEU:HD23	1:C:954:LEU:HA	1.82	0.43
1:A:742:THR:HG22	1:A:744:GLU:H	1.83	0.43
1:C:614:TYR:CD2	1:C:656:PRO:HG3	2.53	0.43
1:B:889:LEU:HD23	1:B:889:LEU:HA	1.77	0.43
1:B:907:ARG:HH21	1:B:915:VAL:HG21	1.83	0.43
1:C:162:LYS:HB3	1:C:162:LYS:HE2	1.78	0.43
1:C:165:THR:HG23	1:C:277:PRO:O	2.18	0.43
1:B:229:THR:HG23	1:B:231:PRO:HA	2.01	0.43
1:B:298:GLU:OE2	1:B:301:ARG:NH1	2.51	0.43
1:C:130:GLU:O	1:C:649:HIS:HB3	2.16	0.43
1:A:922:SER:OG	1:A:923:LYS:N	2.52	0.43
1:B:106:ASN:O	1:B:110:GLU:HG3	2.19	0.43
1:C:948:LEU:HD23	1:C:948:LEU:HA	1.82	0.43
1:C:185:LYS:O	1:C:189:ILE:HG13	2.19	0.43
1:A:57:VAL:CG1	1:A:101:MET:HE1	2.49	0.43
1:C:107:LEU:O	1:C:111:VAL:HG23	2.19	0.43
1:A:130:GLU:O	1:A:649:HIS:HB3	2.19	0.42
1:B:315:TYR:OH	1:B:439:VAL:HA	2.18	0.42
1:C:602:LYS:HG3	1:C:773:TRP:CD1	2.54	0.42
1:C:64:SER:OG	1:C:896:THR:OG1	2.33	0.42
1:A:361:ILE:HG21	1:A:369:VAL:HA	2.01	0.42
1:C:640:THR:HB	1:C:651:ALA:HB1	2.00	0.42
1:A:19:LEU:HD23	1:A:889:LEU:HD23	2.00	0.42
1:B:182:LEU:HD12	1:B:182:LEU:HA	1.65	0.42
1:C:260:ASP:CG	1:C:437:ARG:HH22	2.25	0.42
1:C:708:GLU:HG3	1:C:807:MET:HE2	2.00	0.42
1:B:895:THR:O	1:B:898:ASN:HB2	2.20	0.42
1:C:201:ILE:HD12	1:C:201:ILE:HA	1.74	0.42
1:C:637[A]:ARG:NH2	1:C:671:GLU:OE2	2.34	0.42
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.82	0.42
1:C:182:LEU:HD12	1:C:185:LYS:HD2	2.01	0.42
1:A:560:LEU:HD13	1:A:594:MET:SD	2.60	0.42
1:B:284:TRP:CH2	1:B:594:MET:HE1	2.55	0.42
1:B:306:LEU:O	1:B:310:MET:HG3	2.20	0.42
1:A:738:PHE:O	1:A:742:THR:HB	2.19	0.41
1:C:664:LEU:HG	1:C:666:VAL:HG23	2.02	0.41
1:A:709:TRP:HZ2	1:A:810:ASP:OD2	2.02	0.41
1:B:48:LEU:HD13	1:B:222:ARG:HD3	2.02	0.41
1:C:640:THR:HB	1:C:651:ALA:CB	2.50	0.41
1:A:716:MET:HB3	1:A:793:ALA:HB1	2.02	0.41
1:A:938:LEU:HD11	1:B:329:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:HIS:O	1:B:390:SER:HB2	2.19	0.41
1:B:740:LEU:HD13	1:B:845:VAL:HA	2.01	0.41
1:B:742:THR:HG21	1:B:776:ALA:HB1	2.02	0.41
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.77	0.41
1:C:209:LEU:HA	1:C:209:LEU:HD23	1.81	0.41
1:C:386:HIS:O	1:C:390:SER:HB2	2.20	0.41
1:C:726:SER:HA	1:C:730:GLN:HB2	2.03	0.41
1:B:226:ILE:HD12	1:B:227:LYS:H	1.84	0.41
1:A:442:PHE:HB3	1:A:446:LEU:HD23	2.03	0.41
1:A:889:LEU:HD23	1:A:889:LEU:HA	1.78	0.41
1:B:133:ALA:HA	1:B:136:GLU:HG2	2.02	0.41
1:C:101:MET:HB3	1:C:893:TYR:CE1	2.56	0.41
1:A:427:ILE:HD11	1:B:218:GLN:HG2	2.01	0.41
1:B:68:GLU:CD	1:B:891:ASP:HB3	2.46	0.41
1:B:614:TYR:CD2	1:B:656:PRO:HG3	2.56	0.41
1:C:97:ALA:HB1	1:C:101:MET:CE	2.51	0.41
1:A:850:TRP:N	1:A:851:PRO:HD2	2.36	0.41
1:B:110:GLU:OE1	1:B:190:ARG:HD3	2.21	0.41
1:C:395:ASP:OD1	1:C:395:ASP:N	2.46	0.41
1:C:613:LEU:HD23	1:C:613:LEU:HA	1.90	0.41
1:C:746:GLU:OE2	1:C:746:GLU:N	2.46	0.41
1:C:906:LYS:HE3	1:C:913:TYR:CD1	2.56	0.41
1:A:66:GLU:OE1	1:A:75:LYS:NZ	2.27	0.41
1:C:770:ALA:O	1:C:774:ILE:HG12	2.21	0.41
1:B:228:ARG:HD2	1:B:228:ARG:N	2.36	0.40
1:B:473:SER:OG	1:B:476:GLU:HG2	2.21	0.40
1:B:640:THR:HG21	1:B:820:VAL:HG23	2.04	0.40
1:B:714:ASP:O	1:B:718:VAL:HG23	2.21	0.40
1:C:48:LEU:HD22	1:C:222:ARG:NH1	2.36	0.40
1:A:664:LEU:HD12	1:A:664:LEU:HA	1.91	0.40
1:A:948:LEU:HD23	1:A:948:LEU:HA	1.87	0.40
1:B:164:GLN:HE22	1:B:691:THR:HG23	1.86	0.40
1:C:714:ASP:O	1:C:718:VAL:HG23	2.21	0.40
1:C:367:TYR:CE1	1:C:419:LEU:HG	2.57	0.40
1:C:621:VAL:HG21	1:C:659:THR:HG22	2.03	0.40
1:A:523:ASP:OD1	1:A:523:ASP:N	2.53	0.40
1:B:713:LEU:HD23	1:B:713:LEU:HA	1.90	0.40
1:C:501:LEU:HD12	1:C:502:PRO:HD2	2.03	0.40
1:C:620:LEU:HA	1:C:620:LEU:HD23	1.89	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:C:228:ARG:NH2	1:C:364:THR:OG1[15_556]	2.14	0.06

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	941/974 (97%)	899 (96%)	36 (4%)	6 (1%)	21	53
1	B	940/974 (96%)	897 (95%)	37 (4%)	6 (1%)	21	53
1	C	945/974 (97%)	902 (95%)	36 (4%)	7 (1%)	18	50
All	All	2826/2922 (97%)	2698 (96%)	109 (4%)	19 (1%)	18	50

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	SER
1	C	25	SER
1	A	25	SER
1	A	226	ILE
1	B	226	ILE
1	B	940	PRO
1	C	226	ILE
1	C	940	PRO
1	A	227	LYS
1	A	940	PRO
1	B	21	PRO
1	A	21	PRO
1	C	200	ASP
1	C	21	PRO
1	C	361	ILE
1	A	230	PRO
1	B	230	PRO
1	C	230	PRO
1	B	361	ILE

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	825/849 (97%)	805 (98%)	20 (2%)	43	67
1	B	825/849 (97%)	808 (98%)	17 (2%)	47	69
1	C	828/849 (98%)	805 (97%)	23 (3%)	38	64
All	All	2478/2547 (97%)	2418 (98%)	60 (2%)	43	67

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	8	LYS
1	A	53	LEU
1	A	57	VAL
1	A	193	LEU
1	A	202	THR
1	A	226	ILE
1	A	321[A]	ASP
1	A	321[B]	ASP
1	A	322	LEU
1	A	361	ILE
1	A	376	ASP
1	A	473	SER
1	A	523	ASP
1	A	608	SER
1	A	640	THR
1	A	671	GLU
1	A	700	ARG
1	A	742	THR
1	A	936	ILE
1	B	6	LEU
1	B	26	GLU
1	B	70	LYS
1	B	119	ILE
1	B	193	LEU
1	B	202	THR

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Mol	Chain	Res	Type
1	B	226	ILE
1	B	322	LEU
1	B	328	MET
1	B	376	ASP
1	B	473	SER
1	B	523	ASP
1	B	546	GLN
1	B	671	GLU
1	B	742	THR
1	B	888	ARG
1	B	936	ILE
1	C	6	LEU
1	C	26	GLU
1	C	84	THR
1	C	179	ARG
1	C	193	LEU
1	C	202	THR
1	C	226	ILE
1	C	306	LEU
1	C	321[A]	ASP
1	C	321[B]	ASP
1	C	322	LEU
1	C	384	ARG
1	C	473	SER
1	C	523	ASP
1	C	608	SER
1	C	640	THR
1	C	671	GLU
1	C	700	ARG
1	C	742	THR
1	C	888	ARG
1	C	907	ARG
1	C	924	GLU
1	C	936	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	HIS
1	A	675	GLN
1	B	71	HIS
1	B	468	HIS

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Mol	Chain	Res	Type
1	B	901	GLN
1	C	58	GLN
1	C	669	GLN
1	C	814	HIS

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	944/974 (96%)	-0.00	27 (2%)	53 35	55, 125, 213, 313	3 (0%)
1	B	943/974 (96%)	0.10	34 (3%)	46 29	60, 128, 202, 299	3 (0%)
1	C	947/974 (97%)	-0.08	20 (2%)	63 43	39, 94, 179, 296	4 (0%)
All	All	2834/2922 (96%)	0.00	81 (2%)	53 35	39, 117, 202, 313	10 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	SER	4.4
1	B	133	ALA	4.2
1	A	177	SER	4.1
1	A	752	ILE	4.1
1	A	180	ARG	3.7
1	A	330	ARG	3.7
1	B	119	ILE	3.5
1	A	228	ARG	3.5
1	B	597[A]	TYR	3.4
1	A	923	LYS	3.4
1	C	922	SER	3.3
1	A	176	GLN	3.3
1	B	752	ILE	3.3
1	C	925	ILE	3.3
1	B	242	SER	3.3
1	B	180	ARG	3.2
1	A	965	ASN	3.2
1	C	597[A]	TYR	3.2
1	C	752	ILE	3.2
1	A	882	TYR	3.2
1	C	119	ILE	3.1
1	B	359	LYS	3.1
1	B	177	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	119	ILE	3.0
1	A	6	LEU	2.9
1	C	754	SER	2.9
1	A	754	SER	2.9
1	B	390	SER	2.9
1	B	760	LYS	2.9
1	B	755	ARG	2.8
1	A	931	PRO	2.8
1	B	178	VAL	2.8
1	B	761	PRO	2.7
1	A	359	LYS	2.7
1	A	597[A]	TYR	2.7
1	B	640	THR	2.7
1	B	240	GLY	2.7
1	B	122	LEU	2.6
1	C	359	LYS	2.6
1	B	931	PRO	2.6
1	A	178	VAL	2.6
1	C	134	THR	2.6
1	B	754	SER	2.5
1	C	965	ASN	2.5
1	B	764	GLY	2.4
1	C	22	GLY	2.4
1	B	911	PRO	2.4
1	A	967	GLY	2.4
1	C	226	ILE	2.4
1	B	181	SER	2.4
1	C	924	GLU	2.4
1	A	760	LYS	2.3
1	B	671	GLU	2.3
1	A	494	ARG	2.3
1	B	228	ARG	2.3
1	C	911	PRO	2.3
1	B	360	SER	2.3
1	B	965	ASN	2.3
1	C	184	GLN	2.3
1	B	672	VAL	2.3
1	C	242	SER	2.3
1	A	231	PRO	2.3
1	B	245	HIS	2.3
1	B	403	ILE	2.2
1	A	122	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	6	LEU	2.2
1	A	310	MET	2.2
1	B	644	GLY	2.2
1	B	967	GLY	2.2
1	C	230	PRO	2.2
1	C	330	ARG	2.2
1	B	27	ASP	2.2
1	B	524	SER	2.1
1	A	183	LEU	2.1
1	B	923	LYS	2.1
1	A	966	THR	2.1
1	A	20	VAL	2.1
1	A	935	LEU	2.1
1	C	967	GLY	2.0
1	A	919	PRO	2.0
1	B	246	GLU	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.