



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:59 PM UTC

PDB ID : 4C5U / pdb_00004c5u
Title : Structural Investigations into the Stereochemistry and Activity of a Phenylalanine-2,3-Aminomutase from *Taxus chinensis*
Authors : Wybenga, G.G.; Szymanski, W.; Wu, B.; Feringa, B.L.; Janssen, D.B.; Dijkstra, B.W.
Deposited on : 2013-09-16
Resolution : 2.19 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

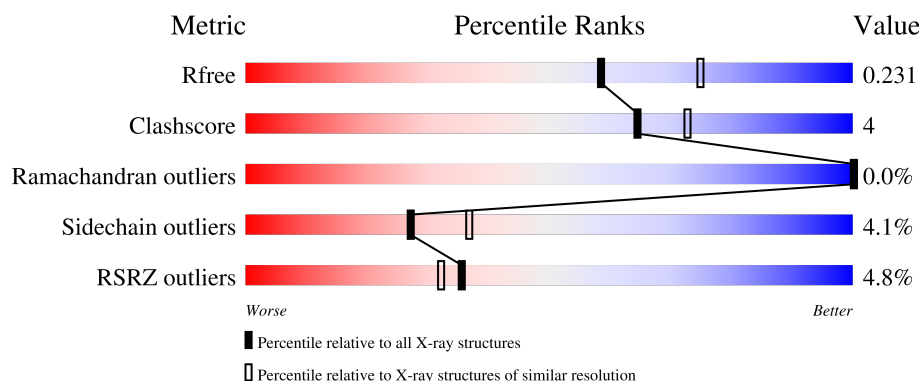
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	707	4% 77% 13% • 9%
1	B	707	3% 80% 9% • 10%
1	C	707	6% 78% 11% • 10%
1	D	707	4% 78% 12% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19779 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 PHENYLALANINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			4962	3147	855	937	23			
1	B	636	Total	C	N	O	S	0	0	0
			4922	3120	847	932	23			
1	C	639	Total	C	N	O	S	0	0	0
			4941	3133	853	932	23			
1	D	636	Total	C	N	O	S	0	0	0
			4917	3121	848	925	23			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q68G84
A	-18	GLY	-	expression tag	UNP Q68G84
A	-17	SER	-	expression tag	UNP Q68G84
A	-16	SER	-	expression tag	UNP Q68G84
A	-15	HIS	-	expression tag	UNP Q68G84
A	-14	HIS	-	expression tag	UNP Q68G84
A	-13	HIS	-	expression tag	UNP Q68G84
A	-12	HIS	-	expression tag	UNP Q68G84
A	-11	HIS	-	expression tag	UNP Q68G84
A	-10	HIS	-	expression tag	UNP Q68G84
A	-9	SER	-	expression tag	UNP Q68G84
A	-8	SER	-	expression tag	UNP Q68G84
A	-7	GLY	-	expression tag	UNP Q68G84
A	-6	LEU	-	expression tag	UNP Q68G84
A	-5	VAL	-	expression tag	UNP Q68G84
A	-4	PRO	-	expression tag	UNP Q68G84
A	-3	ARG	-	expression tag	UNP Q68G84
A	-2	GLY	-	expression tag	UNP Q68G84
A	-1	SER	-	expression tag	UNP Q68G84
A	0	HIS	-	expression tag	UNP Q68G84
A	322	ALA	TYR	engineered mutation	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q68G84
B	-18	GLY	-	expression tag	UNP Q68G84
B	-17	SER	-	expression tag	UNP Q68G84
B	-16	SER	-	expression tag	UNP Q68G84
B	-15	HIS	-	expression tag	UNP Q68G84
B	-14	HIS	-	expression tag	UNP Q68G84
B	-13	HIS	-	expression tag	UNP Q68G84
B	-12	HIS	-	expression tag	UNP Q68G84
B	-11	HIS	-	expression tag	UNP Q68G84
B	-10	HIS	-	expression tag	UNP Q68G84
B	-9	SER	-	expression tag	UNP Q68G84
B	-8	SER	-	expression tag	UNP Q68G84
B	-7	GLY	-	expression tag	UNP Q68G84
B	-6	LEU	-	expression tag	UNP Q68G84
B	-5	VAL	-	expression tag	UNP Q68G84
B	-4	PRO	-	expression tag	UNP Q68G84
B	-3	ARG	-	expression tag	UNP Q68G84
B	-2	GLY	-	expression tag	UNP Q68G84
B	-1	SER	-	expression tag	UNP Q68G84
B	0	HIS	-	expression tag	UNP Q68G84
B	322	ALA	TYR	engineered mutation	UNP Q68G84
C	-19	MET	-	expression tag	UNP Q68G84
C	-18	GLY	-	expression tag	UNP Q68G84
C	-17	SER	-	expression tag	UNP Q68G84
C	-16	SER	-	expression tag	UNP Q68G84
C	-15	HIS	-	expression tag	UNP Q68G84
C	-14	HIS	-	expression tag	UNP Q68G84
C	-13	HIS	-	expression tag	UNP Q68G84
C	-12	HIS	-	expression tag	UNP Q68G84
C	-11	HIS	-	expression tag	UNP Q68G84
C	-10	HIS	-	expression tag	UNP Q68G84
C	-9	SER	-	expression tag	UNP Q68G84
C	-8	SER	-	expression tag	UNP Q68G84
C	-7	GLY	-	expression tag	UNP Q68G84
C	-6	LEU	-	expression tag	UNP Q68G84
C	-5	VAL	-	expression tag	UNP Q68G84
C	-4	PRO	-	expression tag	UNP Q68G84
C	-3	ARG	-	expression tag	UNP Q68G84
C	-2	GLY	-	expression tag	UNP Q68G84
C	-1	SER	-	expression tag	UNP Q68G84
C	0	HIS	-	expression tag	UNP Q68G84
C	322	ALA	TYR	engineered mutation	UNP Q68G84

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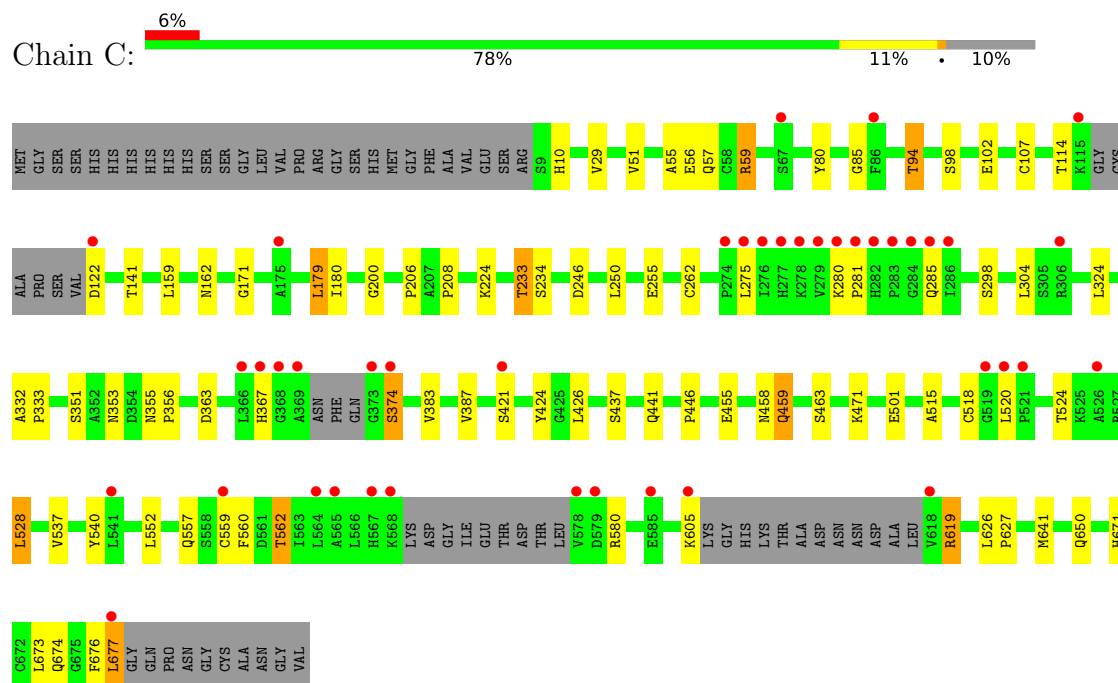
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP Q68G84
D	-18	GLY	-	expression tag	UNP Q68G84
D	-17	SER	-	expression tag	UNP Q68G84
D	-16	SER	-	expression tag	UNP Q68G84
D	-15	HIS	-	expression tag	UNP Q68G84
D	-14	HIS	-	expression tag	UNP Q68G84
D	-13	HIS	-	expression tag	UNP Q68G84
D	-12	HIS	-	expression tag	UNP Q68G84
D	-11	HIS	-	expression tag	UNP Q68G84
D	-10	HIS	-	expression tag	UNP Q68G84
D	-9	SER	-	expression tag	UNP Q68G84
D	-8	SER	-	expression tag	UNP Q68G84
D	-7	GLY	-	expression tag	UNP Q68G84
D	-6	LEU	-	expression tag	UNP Q68G84
D	-5	VAL	-	expression tag	UNP Q68G84
D	-4	PRO	-	expression tag	UNP Q68G84
D	-3	ARG	-	expression tag	UNP Q68G84
D	-2	GLY	-	expression tag	UNP Q68G84
D	-1	SER	-	expression tag	UNP Q68G84
D	0	HIS	-	expression tag	UNP Q68G84
D	322	ALA	TYR	engineered mutation	UNP Q68G84

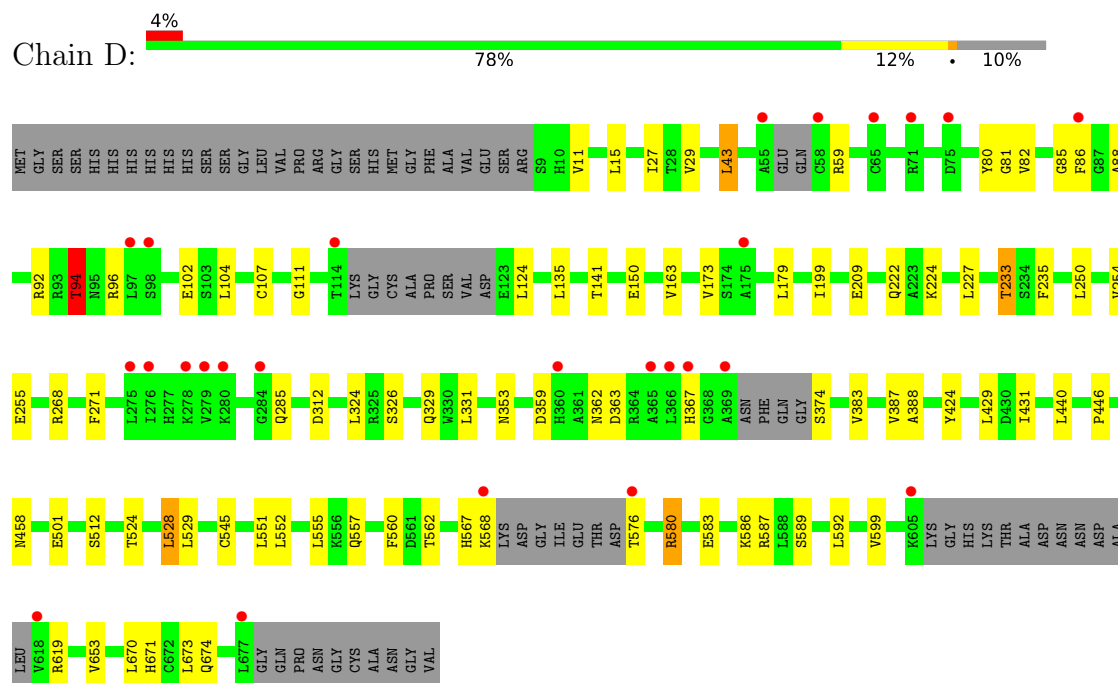
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	6	Total	O	0	0
			6	6		
2	C	10	Total	O	0	0
			10	10		
2	D	6	Total	O	0	0
			6	6		

• Molecule 1: PHENYLALANINE AMMONIA-LYASE



• Molecule 1: PHENYLALANINE AMMONIA-LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.48Å 147.27Å 99.77Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	48.38 – 2.19 48.38 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.38-2.19) 98.1 (48.38-2.19)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.189 , 0.224 0.192 , 0.231	Depositor DCC
R_{free} test set	7178 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.865 for H, K, L 0.135 for L, -K, H	Depositor
Outliers	1 of 141777 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19779	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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

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	0.80	0/5045	0.94	4/6843 (0.1%)
1	B	0.75	0/5002	0.93	0/6782
1	C	0.77	0/5024	0.92	4/6813 (0.1%)
1	D	0.78	0/4999	0.92	3/6780 (0.0%)
All	All	0.78	0/20070	0.93	11/27218 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	VAL	CB-CA-C	-6.04	103.71	111.20
1	A	490	MET	N-CA-C	5.71	117.51	111.28
1	A	273	HIS	CA-C-N	5.60	125.97	119.47
1	A	273	HIS	C-N-CA	5.60	125.97	119.47
1	C	233	THR	CB-CA-C	5.56	120.97	111.46
1	C	281	PRO	N-CA-C	5.46	119.86	112.48
1	D	94	THR	N-CA-C	5.36	116.42	108.60
1	C	234	SER	N-CA-C	5.27	117.02	111.28
1	D	592	LEU	N-CA-C	5.17	116.60	111.07
1	C	94	THR	CB-CA-C	-5.11	99.47	110.45
1	A	233	THR	CB-CA-C	5.10	120.58	110.42

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	4962	0	5044	52	0
1	B	4922	0	4993	43	0
1	C	4941	0	5021	46	0
1	D	4917	0	5004	40	0
2	A	15	0	0	0	0
2	B	6	0	0	0	0
2	C	10	0	0	0	0
2	D	6	0	0	0	0
All	All	19779	0	20062	156	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 4.

All (156) 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:29:VAL:HG12	1:A:141:THR:HG21	1.58	0.85
1:D:580:ARG:HH11	1:D:580:ARG:CG	2.01	0.74
1:A:80:TYR:HB3	1:A:367:HIS:HD2	1.52	0.73
1:B:671:HIS:O	1:B:674:GLN:HG2	1.89	0.72
1:D:29:VAL:HG12	1:D:141:THR:HG21	1.71	0.71
1:B:380:MET:HA	1:B:380:MET:HE2	1.73	0.71
1:B:446:PRO:HD3	1:D:446:PRO:HD3	1.72	0.71
1:A:557:GLN:NE2	1:D:557:GLN:OE1	2.21	0.71
1:C:501:GLU:OE1	1:C:619:ARG:HD2	1.91	0.70
1:B:557:GLN:NE2	1:C:557:GLN:OE1	2.23	0.69
1:A:650:GLN:HG3	1:B:111:GLY:O	1.93	0.68
1:A:80:TYR:HB3	1:A:367:HIS:CD2	2.30	0.66
1:C:224:LYS:HE2	1:C:356:PRO:HD2	1.78	0.65
1:A:43:LEU:HD22	1:A:134:LEU:HD22	1.79	0.64
1:B:224:LYS:HE2	1:B:356:PRO:HD2	1.80	0.63
1:C:515:ALA:HA	1:C:520:LEU:HD12	1.82	0.61
1:D:163:VAL:HG22	1:D:199:ILE:HG12	1.83	0.61
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.82	0.60
1:C:304:LEU:HD11	1:C:619:ARG:HD3	1.84	0.60
1:B:233:THR:HG21	1:B:373:GLY:N	2.15	0.60
1:C:437:SER:O	1:C:441:GLN:HG2	2.02	0.59
1:B:123:GLU:OE1	1:B:166:LYS:HE3	2.05	0.57
1:D:580:ARG:HH11	1:D:580:ARG:HG3	1.68	0.57
1:C:524:THR:HG22	1:C:528:LEU:HD22	1.87	0.56
1:C:29:VAL:HG12	1:C:141:THR:HG21	1.86	0.56
1:C:455:GLU:HB3	1:C:459:GLN:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HD2	1:A:216:LEU:HD21	1.88	0.55
1:C:171:GLY:O	1:C:180:ILE:HD12	2.06	0.55
1:A:374:SER:HA	1:A:463:SER:HB3	1.89	0.54
1:D:82:VAL:HG22	1:D:224:LYS:HB2	1.87	0.54
1:A:501:GLU:OE1	1:A:619:ARG:HD2	2.06	0.54
1:A:446:PRO:HD3	1:C:446:PRO:HD3	1.90	0.54
1:D:671:HIS:O	1:D:674:GLN:HG2	2.08	0.54
1:D:501:GLU:OE1	1:D:619:ARG:HD2	2.08	0.53
1:A:255:GLU:HG2	1:A:331:LEU:HD13	1.91	0.52
1:A:351:SER:HB2	1:C:280:LYS:HA	1.91	0.52
1:A:88:ALA:HB2	1:A:458:ASN:HB2	1.90	0.52
1:A:424:TYR:OH	1:B:85:GLY:HA2	2.10	0.52
1:A:380:MET:HA	1:A:380:MET:HE2	1.92	0.52
1:A:427:LYS:NZ	1:B:455:GLU:OE2	2.40	0.52
1:A:81:GLY:HA3	1:A:227:LEU:HD22	1.92	0.52
1:A:551:LEU:O	1:A:555:LEU:HG	2.10	0.52
1:D:233:THR:HG23	1:D:233:THR:O	2.10	0.51
1:A:321:ARG:HG2	1:C:458:ASN:HA	1.93	0.50
1:C:179:LEU:HD23	1:D:431:ILE:HD13	1.94	0.50
1:A:29:VAL:CG1	1:A:141:THR:HG21	2.36	0.50
1:B:334:LEU:HD22	1:B:386:ALA:HA	1.93	0.50
1:B:327:SER:OG	1:B:328:PRO:HD3	2.12	0.50
1:D:94:THR:HB	1:D:96:ARG:H	1.77	0.50
1:B:265:ILE:HG21	1:B:324:LEU:HD12	1.94	0.49
1:B:388:ALA:HA	1:B:440:LEU:HG	1.94	0.49
1:C:80:TYR:HB3	1:C:367:HIS:CD2	2.48	0.49
1:C:114:THR:OG1	1:C:122:ASP:HB2	2.12	0.49
1:D:285:GLN:CD	1:D:329:GLN:HG3	2.38	0.49
1:B:15:LEU:HD21	1:B:673:LEU:HD23	1.95	0.49
1:C:285:GLN:HB2	1:C:332:ALA:HB2	1.95	0.49
1:A:332:ALA:HB3	1:A:333:PRO:CD	2.42	0.49
1:C:374:SER:HA	1:C:463:SER:HB2	1.95	0.49
1:B:437:SER:O	1:B:441:GLN:HG2	2.13	0.48
1:D:88:ALA:HB2	1:D:458:ASN:HB2	1.94	0.48
1:A:545:CYS:SG	1:A:589:SER:HA	2.54	0.48
1:A:334:LEU:HD22	1:A:386:ALA:HA	1.95	0.48
1:C:671:HIS:O	1:C:674:GLN:HG2	2.14	0.48
1:C:332:ALA:HB3	1:C:333:PRO:HD3	1.94	0.48
1:B:27:ILE:CD1	1:B:43:LEU:HB2	2.43	0.48
1:B:329:GLN:O	1:D:374:SER:OG	2.27	0.48
1:A:437:SER:O	1:A:441:GLN:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ILE:CD1	1:D:43:LEU:HB2	2.44	0.47
1:C:10:HIS:HE2	1:C:255:GLU:CD	2.21	0.47
1:A:267:GLY:HA3	1:A:324:LEU:HD11	1.96	0.47
1:A:560:PHE:HB2	1:D:560:PHE:HB2	1.96	0.47
1:C:424:TYR:OH	1:D:85:GLY:HA2	2.14	0.47
1:A:579:ASP:OD1	1:D:567:HIS:NE2	2.42	0.47
1:B:501:GLU:OE1	1:B:619:ARG:HD2	2.14	0.47
1:D:429:LEU:HD21	1:D:653:VAL:HG21	1.96	0.47
1:B:131:SER:HB2	1:B:238:ALA:HB1	1.97	0.47
1:A:388:ALA:HA	1:A:440:LEU:HG	1.97	0.47
1:C:383:VAL:O	1:C:387:VAL:HG23	2.14	0.46
1:A:567:HIS:O	1:A:568:LYS:HD3	2.15	0.46
1:B:24:VAL:HG21	1:B:39:HIS:HD2	1.80	0.46
1:A:94:THR:HG23	1:B:421:SER:OG	2.16	0.46
1:D:81:GLY:HA3	1:D:227:LEU:HD22	1.98	0.46
1:B:59:ARG:HD2	1:B:63:GLU:OE1	2.16	0.46
1:A:419:ASP:OD2	1:B:96:ARG:NH1	2.47	0.46
1:D:86:PHE:CD2	1:D:104:LEU:HD13	2.51	0.46
1:A:596:MET:O	1:A:599:VAL:HG12	2.16	0.46
1:C:304:LEU:CD1	1:C:619:ARG:HD3	2.45	0.46
1:A:27:ILE:CD1	1:A:43:LEU:HB2	2.47	0.45
1:A:181:PRO:HB2	1:A:235:PHE:CD2	2.51	0.45
1:C:518:CYS:O	1:C:580:ARG:HD3	2.16	0.45
1:D:268:ARG:O	1:D:271:PHE:HD1	1.99	0.45
1:B:181:PRO:HB2	1:B:235:PHE:CD2	2.51	0.45
1:B:369:ALA:CB	1:D:326:SER:HB3	2.46	0.45
1:A:500:GLU:HG3	1:A:537:VAL:HG12	1.97	0.45
1:C:246:ASP:O	1:C:250:LEU:HG	2.16	0.45
1:C:559:CYS:O	1:C:562:THR:HG22	2.16	0.45
1:D:359:ASP:OD2	1:D:362:ASN:HB2	2.17	0.45
1:A:80:TYR:CB	1:A:367:HIS:CD2	3.00	0.45
1:A:163:VAL:HG22	1:A:199:ILE:HG23	1.99	0.44
1:A:224:LYS:O	1:A:224:LYS:HG2	2.18	0.44
1:A:374:SER:HA	1:A:463:SER:CB	2.47	0.44
1:B:560:PHE:CE1	1:C:559:CYS:HB3	2.52	0.44
1:D:383:VAL:O	1:D:387:VAL:HG23	2.17	0.44
1:C:332:ALA:HB3	1:C:333:PRO:CD	2.47	0.44
1:C:51:VAL:HG21	1:C:159:LEU:HD13	2.00	0.44
1:D:11:VAL:O	1:D:15:LEU:HG	2.18	0.44
1:B:560:PHE:HB2	1:C:560:PHE:HB2	2.00	0.44
1:C:421:SER:HB3	1:D:92:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:VAL:HA	1:C:540:TYR:CE2	2.53	0.43
1:B:27:ILE:HD12	1:B:43:LEU:HB2	2.01	0.43
1:A:111:GLY:O	1:B:650:GLN:HG3	2.17	0.43
1:B:268:ARG:O	1:B:271:PHE:HD1	2.01	0.43
1:C:206:PRO:HB2	1:C:208:PRO:HD2	1.99	0.43
1:B:309:TYR:O	1:B:313:LYS:HG3	2.19	0.43
1:D:524:THR:HG22	1:D:528:LEU:HD22	2.01	0.43
1:C:426:LEU:HD11	1:C:641:MET:SD	2.58	0.43
1:A:131:SER:CB	1:A:238:ALA:HB1	2.49	0.43
1:D:388:ALA:HA	1:D:440:LEU:HG	2.01	0.43
1:D:512:SER:HB2	1:D:529:LEU:HD21	2.00	0.43
1:A:82:VAL:HG22	1:A:224:LYS:HB2	2.01	0.43
1:D:545:CYS:SG	1:D:589:SER:HA	2.58	0.43
1:A:80:TYR:CB	1:A:367:HIS:HD2	2.27	0.42
1:B:626:LEU:HB3	1:B:627:PRO:HD3	2.01	0.42
1:B:324:LEU:C	1:B:324:LEU:HD23	2.44	0.42
1:C:355:ASN:OD1	1:C:356:PRO:HA	2.19	0.42
1:C:55:ALA:O	1:C:59:ARG:HB3	2.20	0.42
1:A:233:THR:HG23	1:A:233:THR:O	2.20	0.42
1:B:285:GLN:CD	1:B:329:GLN:HG3	2.45	0.42
1:B:307:GLU:O	1:B:311:ILE:HG12	2.19	0.42
1:C:676:PHE:C	1:C:677:LEU:HG	2.45	0.42
1:A:279:VAL:O	1:C:351:SER:HB2	2.18	0.42
1:B:54:GLU:HA	1:B:54:GLU:OE1	2.20	0.41
1:A:332:ALA:O	1:A:336:GLN:HG3	2.20	0.41
1:B:82:VAL:HG22	1:B:224:LYS:HB2	2.01	0.41
1:D:255:GLU:HG2	1:D:331:LEU:HD13	2.03	0.41
1:C:85:GLY:HA2	1:D:424:TYR:OH	2.20	0.41
1:C:262:CYS:HB2	1:C:324:LEU:HD21	2.02	0.41
1:D:124:LEU:HD13	1:D:235:PHE:CE1	2.54	0.41
1:A:626:LEU:HB3	1:A:627:PRO:HD3	2.01	0.41
1:D:250:LEU:O	1:D:254:VAL:HG23	2.21	0.41
1:D:583:GLU:O	1:D:587:ARG:HG3	2.20	0.41
1:A:51:VAL:HG21	1:A:159:LEU:HD13	2.02	0.41
1:A:280:LYS:HA	1:C:351:SER:HB2	2.03	0.41
1:C:626:LEU:N	1:C:627:PRO:HD2	2.36	0.41
1:B:72:LYS:HA	1:B:72:LYS:HD3	1.91	0.41
1:A:33:THR:HA	1:A:34:PRO:HD3	1.87	0.41
1:B:94:THR:HG22	1:B:96:ARG:H	1.85	0.41
1:B:162:ASN:ND2	1:B:200:GLY:HA2	2.36	0.41
1:C:471:LYS:HA	1:C:471:LYS:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:TYR:HB3	1:D:367:HIS:CD2	2.56	0.41
1:D:551:LEU:O	1:D:555:LEU:HG	2.21	0.40
1:C:650:GLN:HG3	1:D:111:GLY:O	2.22	0.40
1:A:65:CYS:O	1:A:69:VAL:HG23	2.20	0.40
1:B:304:LEU:HD11	1:B:619:ARG:HD3	2.04	0.40
1:C:162:ASN:ND2	1:C:200:GLY:HA2	2.37	0.40
1:A:224:LYS:HE2	1:A:356:PRO:HD2	2.04	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	631/707 (89%)	616 (98%)	14 (2%)	1 (0%)	43	51
1	B	622/707 (88%)	603 (97%)	19 (3%)	0	100	100
1	C	629/707 (89%)	609 (97%)	20 (3%)	0	100	100
1	D	624/707 (88%)	610 (98%)	14 (2%)	0	100	100
All	All	2506/2828 (89%)	2438 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ALA

5.3.2 Protein sidechains [i](#)

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	543/592 (92%)	517 (95%)	26 (5%)	23	30
1	B	538/592 (91%)	522 (97%)	16 (3%)	36	49
1	C	539/592 (91%)	517 (96%)	22 (4%)	27	37
1	D	537/592 (91%)	512 (95%)	25 (5%)	23	31
All	All	2157/2368 (91%)	2068 (96%)	89 (4%)	27	37

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	57	GLN
1	A	59	ARG
1	A	84	THR
1	A	92	ARG
1	A	94	THR
1	A	102	GLU
1	A	107	CYS
1	A	162	ASN
1	A	166	LYS
1	A	179	LEU
1	A	202	ASP
1	A	209	GLU
1	A	233	THR
1	A	253	LEU
1	A	324	LEU
1	A	353	ASN
1	A	374	SER
1	A	455	GLU
1	A	528	LEU
1	A	562	THR
1	A	564	LEU
1	A	575	ASP
1	A	640	VAL
1	A	673	LEU
1	A	674	GLN
1	B	43	LEU
1	B	59	ARG
1	B	63	GLU
1	B	94	THR

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Mol	Chain	Res	Type
1	B	102	GLU
1	B	107	CYS
1	B	135	LEU
1	B	179	LEU
1	B	233	THR
1	B	243	VAL
1	B	312	ASP
1	B	374	SER
1	B	528	LEU
1	B	562	THR
1	B	618	VAL
1	B	673	LEU
1	C	56	GLU
1	C	57	GLN
1	C	59	ARG
1	C	94	THR
1	C	98	SER
1	C	102	GLU
1	C	107	CYS
1	C	179	LEU
1	C	233	THR
1	C	275	LEU
1	C	298	SER
1	C	353	ASN
1	C	363	ASP
1	C	374	SER
1	C	459	GLN
1	C	528	LEU
1	C	552	LEU
1	C	562	THR
1	C	605	LYS
1	C	619	ARG
1	C	673	LEU
1	C	677	LEU
1	D	43	LEU
1	D	59	ARG
1	D	94	THR
1	D	102	GLU
1	D	107	CYS
1	D	135	LEU
1	D	150	GLU
1	D	179	LEU

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Mol	Chain	Res	Type
1	D	209	GLU
1	D	222	GLN
1	D	233	THR
1	D	312	ASP
1	D	324	LEU
1	D	353	ASN
1	D	363	ASP
1	D	528	LEU
1	D	552	LEU
1	D	562	THR
1	D	568	LYS
1	D	576	THR
1	D	580	ARG
1	D	586	LYS
1	D	599	VAL
1	D	670	LEU
1	D	673	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	57	GLN
1	A	277	HIS
1	A	285	GLN
1	A	336	GLN
1	A	360	HIS
1	A	459	GLN
1	A	557	GLN
1	B	47	HIS
1	B	57	GLN
1	B	162	ASN
1	B	277	HIS
1	B	285	GLN
1	B	336	GLN
1	B	360	HIS
1	B	450	HIS
1	B	462	ASN
1	C	47	HIS
1	C	353	ASN
1	C	362	ASN
1	C	413	ASN

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Mol	Chain	Res	Type
1	C	462	ASN
1	D	22	ASN
1	D	231	ASN
1	D	367	HIS
1	D	456	GLN
1	D	557	GLN
1	D	674	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	641/707 (90%)	0.21	31 (4%)	35	32	20, 37, 61, 92	0
1	B	636/707 (89%)	0.29	23 (3%)	46	43	20, 40, 66, 81	0
1	C	639/707 (90%)	0.35	42 (6%)	24	21	19, 39, 72, 93	0
1	D	636/707 (89%)	0.32	26 (4%)	41	38	20, 39, 64, 85	0
All	All	2552/2828 (90%)	0.29	122 (4%)	35	32	19, 39, 66, 93	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ILE	8.1
1	B	276	ILE	6.2
1	C	369	ALA	5.9
1	C	281	PRO	5.5
1	A	121	VAL	5.2
1	B	677	LEU	5.1
1	C	677	LEU	4.9
1	C	278	LYS	4.9
1	D	55	ALA	4.6
1	D	369	ALA	4.6
1	C	275	LEU	4.5
1	C	280	LYS	4.4
1	A	276	ILE	4.3
1	D	568	LYS	4.2
1	A	367	HIS	4.2
1	B	575	ASP	4.1
1	C	277	HIS	4.1
1	A	115	LYS	4.1
1	B	115	LYS	4.0
1	A	86	PHE	4.0
1	A	32	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	279	VAL	3.9
1	D	677	LEU	3.9
1	A	677	LEU	3.7
1	B	618	VAL	3.7
1	C	282	HIS	3.5
1	C	86	PHE	3.5
1	D	367	HIS	3.3
1	A	279	VAL	3.3
1	D	576	THR	3.2
1	D	175	ALA	3.2
1	B	284	GLY	3.2
1	C	568	LYS	3.2
1	B	566	LEU	3.1
1	A	284	GLY	3.1
1	D	618	VAL	3.1
1	C	373	GLY	3.0
1	B	277	HIS	3.0
1	C	526	ALA	3.0
1	D	275	LEU	3.0
1	D	279	VAL	3.0
1	A	568	LYS	3.0
1	A	278	LYS	3.0
1	B	519	GLY	3.0
1	C	286	ILE	3.0
1	A	275	LEU	2.9
1	B	285	GLN	2.9
1	D	360	HIS	2.9
1	A	281	PRO	2.9
1	C	285	GLN	2.8
1	A	575	ASP	2.8
1	D	280	LYS	2.8
1	C	578	VAL	2.8
1	A	373	GLY	2.8
1	D	284	GLY	2.8
1	B	55	ALA	2.7
1	C	175	ALA	2.7
1	C	565	ALA	2.7
1	D	278	LYS	2.7
1	D	71	ARG	2.7
1	A	139	SER	2.6
1	B	283	PRO	2.6
1	D	114	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	276	ILE	2.5
1	A	671	HIS	2.5
1	C	579	ASP	2.5
1	B	281	PRO	2.5
1	C	274	PRO	2.5
1	A	277	HIS	2.5
1	C	618	VAL	2.5
1	A	359	ASP	2.5
1	C	567	HIS	2.5
1	B	76	GLY	2.5
1	C	283	PRO	2.4
1	B	364	ARG	2.4
1	A	358	ILE	2.4
1	A	605	LYS	2.4
1	A	366	LEU	2.4
1	A	57	GLN	2.4
1	C	67	SER	2.4
1	B	274	PRO	2.4
1	C	541	LEU	2.4
1	C	564	LEU	2.4
1	A	355	ASN	2.4
1	C	368	GLY	2.4
1	C	115	LYS	2.4
1	C	284	GLY	2.3
1	B	60	ALA	2.3
1	B	81	GLY	2.3
1	C	374	SER	2.3
1	A	94	THR	2.3
1	B	605	LYS	2.3
1	C	122	ASP	2.3
1	B	275	LEU	2.3
1	A	360	HIS	2.2
1	C	367	HIS	2.2
1	C	585	GLU	2.2
1	D	65	CYS	2.2
1	C	605	LYS	2.2
1	C	366	LEU	2.2
1	A	364	ARG	2.2
1	D	86	PHE	2.2
1	A	363	ASP	2.2
1	D	75	ASP	2.2
1	A	144	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	520	LEU	2.2
1	D	58	CYS	2.2
1	C	421	SER	2.2
1	D	98	SER	2.2
1	C	519	GLY	2.1
1	C	306	ARG	2.1
1	D	366	LEU	2.1
1	B	576	THR	2.1
1	C	521	PRO	2.1
1	A	365	ALA	2.1
1	D	365	ALA	2.1
1	B	577	LEU	2.0
1	C	559	CYS	2.0
1	D	605	LYS	2.0
1	D	97	LEU	2.0
1	A	587	ARG	2.0
1	B	559	CYS	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.