



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:17 PM UTC

PDB ID : 4C6G / pdb_00004c6g
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 : 2013-09-18
Resolution : 2.10 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

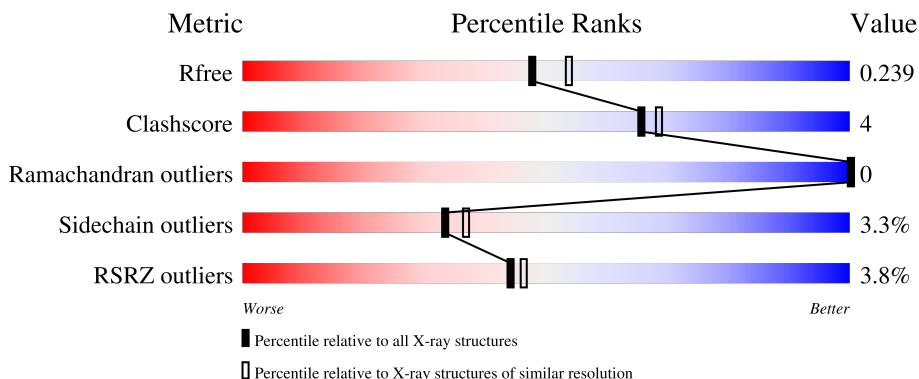
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	
1	B	707	
1	C	707	
1	D	707	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19587 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	624	Total	C	N	O	S	0	0	0
			4833	3074	826	911	22			
1	B	626	Total	C	N	O	S	0	0	0
			4848	3085	828	913	22			
1	C	625	Total	C	N	O	S	0	0	0
			4839	3078	825	914	22			
1	D	626	Total	C	N	O	S	0	0	0
			4847	3083	828	914	22			

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	231	ALA	ASN	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	231	ALA	ASN	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	231	ALA	ASN	engineered mutation	UNP Q68G84

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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	231	ALA	ASN	engineered mutation	UNP Q68G84

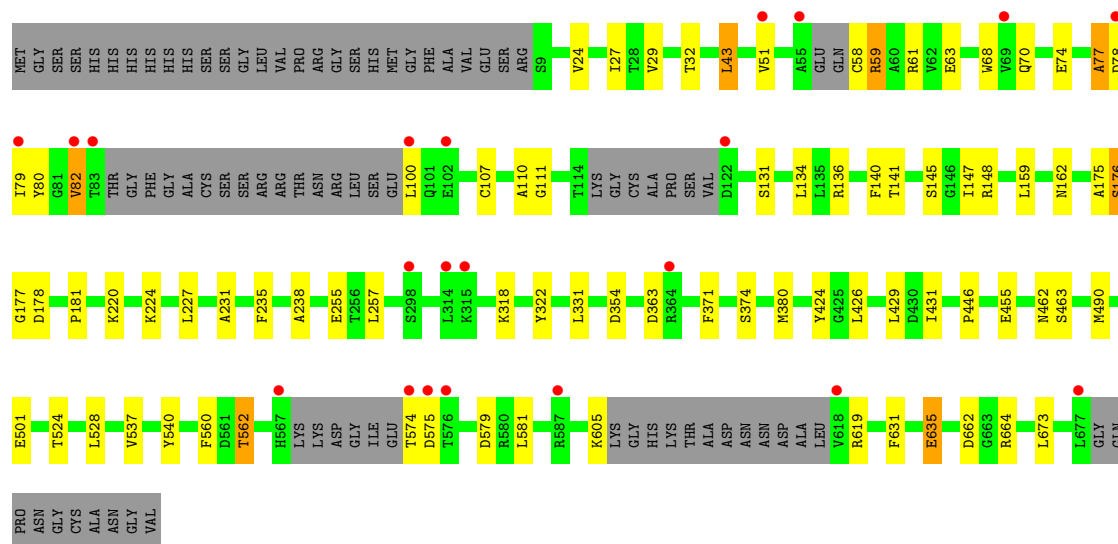
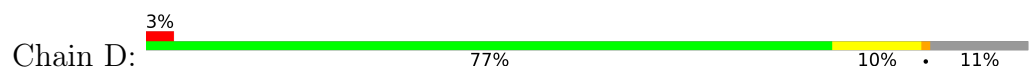
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	42	Total	O	0	0
			42	42		
2	C	60	Total	O	0	0
			60	60		
2	D	45	Total	O	0	0
			45	45		

- Molecule 1: PHENYLALANINE AMMONIA-LYASE



Chain C: 3% 78% 9% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.96Å 146.57Å 99.33Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	48.73 – 2.10 48.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.73-2.10) 99.7 (48.73-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.201 , 0.241 (Not available) , 0.239	Depositor DCC
R_{free} test set	8119 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19587	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.92	2/4916 (0.0%)	0.93	10/6671 (0.1%)
1	B	0.93	2/4932 (0.0%)	0.94	5/6692 (0.1%)
1	C	0.81	4/4921 (0.1%)	0.91	4/6678 (0.1%)
1	D	0.95	2/4930 (0.0%)	0.90	4/6691 (0.1%)
All	All	0.91	10/19699 (0.1%)	0.92	23/26732 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	ALA	C-N	-36.41	0.91	1.33
1	D	77	ALA	C-N	-35.06	0.88	1.33
1	A	77	ALA	C-N	-33.68	0.90	1.33
1	D	78	ASP	C-N	-24.21	1.03	1.33
1	C	71	ARG	CZ-NH2	19.95	1.59	1.33
1	B	78	ASP	C-N	-19.80	1.05	1.33
1	A	78	ASP	C-N	-18.91	1.10	1.33
1	C	71	ARG	CZ-NH1	-13.89	1.13	1.32
1	C	71	ARG	NE-CZ	7.89	1.41	1.33
1	C	71	ARG	CD-NE	6.80	1.55	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	ARG	NE-CZ-NH2	-16.13	104.69	119.20
1	B	77	ALA	O-C-N	-15.03	104.32	122.81
1	B	77	ALA	CA-C-N	13.97	141.51	122.79
1	B	77	ALA	C-N-CA	13.97	141.51	122.79
1	D	78	ASP	O-C-N	-12.32	104.63	122.87
1	A	77	ALA	CA-C-N	11.55	141.02	123.23
1	A	77	ALA	C-N-CA	11.55	141.02	123.23
1	A	77	ALA	O-C-N	-10.50	108.29	122.36
1	A	176	SER	N-CA-C	-9.39	102.42	112.93
1	A	78	ASP	CA-C-N	8.79	135.46	122.98
1	A	78	ASP	C-N-CA	8.79	135.46	122.98
1	D	78	ASP	CA-C-N	8.72	135.36	122.98
1	D	78	ASP	C-N-CA	8.72	135.36	122.98
1	B	176	SER	N-CA-C	-8.40	104.07	112.97
1	C	176	SER	N-CA-C	-8.25	103.69	112.93
1	A	78	ASP	O-C-N	-8.03	110.08	122.93
1	A	71	ARG	NE-CZ-NH2	-6.83	113.05	119.20
1	D	176	SER	N-CA-C	-6.36	106.22	112.97
1	C	71	ARG	NE-CZ-NH1	6.27	127.77	121.50
1	C	575	ASP	N-CA-C	-5.63	105.28	111.82
1	A	299	SER	CA-C-N	5.41	124.92	119.19
1	A	299	SER	C-N-CA	5.41	124.92	119.19
1	B	167	VAL	N-CA-C	5.35	113.97	107.61

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	71	ARG	Sidechain
1	D	77	ALA	Mainchain

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	4833	0	4901	30	0
1	B	4848	0	4913	48	0
1	C	4839	0	4911	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4847	0	4917	45	0
2	A	73	0	0	0	0
2	B	42	0	0	0	0
2	C	60	0	0	0	0
2	D	45	0	0	0	0
All	All	19587	0	19642	148	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 (148) 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:80:TYR:HB3	1:B:318:LYS:HG2	1.58	0.85
1:C:80:TYR:CB	1:D:318:LYS:HG2	2.09	0.81
1:C:304:LEU:HD11	1:C:619:ARG:HD3	1.64	0.80
1:A:80:TYR:CB	1:B:318:LYS:HG2	2.11	0.80
1:C:80:TYR:HB3	1:D:318:LYS:HG2	1.67	0.77
1:C:501:GLU:OE1	1:C:619:ARG:HD2	1.86	0.74
1:C:99:GLU:HA	1:C:102:GLU:HG2	1.76	0.67
1:B:552:LEU:O	1:B:556:LYS:HG3	1.94	0.66
1:C:574:THR:HG23	1:C:575:ASP:N	2.11	0.66
1:D:70:GLN:O	1:D:74:GLU:HG2	1.98	0.64
1:A:662:ASP:OD1	1:A:664:ARG:HD3	1.99	0.63
1:A:176:SER:HB3	1:B:322:TYR:OH	1.99	0.62
1:C:176:SER:HB3	1:D:322:TYR:OH	2.00	0.61
1:C:418:PRO:O	1:C:542:GLU:HB2	2.00	0.61
1:C:318:LYS:HG2	1:D:80:TYR:HB2	1.82	0.61
1:C:322:TYR:OH	1:D:176:SER:HB3	2.00	0.60
1:A:175:ALA:C	1:A:177:GLY:H	2.11	0.58
1:C:162:ASN:HD22	1:C:200:GLY:HA2	1.68	0.57
1:D:255:GLU:HG2	1:D:331:LEU:HD13	1.86	0.57
1:D:231:ALA:O	1:D:354:ASP:HA	2.03	0.57
1:A:43:LEU:HD22	1:A:134:LEU:HD22	1.87	0.56
1:B:231:ALA:HB1	1:B:371:PHE:HD2	1.70	0.56
1:B:557:GLN:OE1	1:C:557:GLN:NE2	2.37	0.56
1:C:446:PRO:HD3	1:D:446:PRO:HD3	1.88	0.55
1:C:574:THR:HG23	1:C:575:ASP:H	1.71	0.55
1:B:27:ILE:CD1	1:B:43:LEU:HB2	2.36	0.55
1:D:131:SER:HB2	1:D:238:ALA:HB1	1.89	0.55
1:D:43:LEU:HD22	1:D:134:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:LYS:HG2	1:D:80:TYR:CB	2.37	0.55
1:C:437:SER:O	1:C:441:GLN:HG2	2.07	0.54
1:B:224:LYS:HE2	1:B:356:PRO:HD2	1.88	0.54
1:A:114:THR:HG22	1:C:657:PHE:CZ	2.43	0.53
1:A:70:GLN:OE1	1:A:222:GLN:HB3	2.09	0.52
1:A:231:ALA:O	1:A:354:ASP:HA	2.09	0.52
1:B:429:LEU:HD23	1:D:110:ALA:HB1	1.91	0.52
1:B:501:GLU:OE2	1:B:619:ARG:NH1	2.42	0.52
1:D:58:CYS:HA	1:D:61:ARG:HE	1.74	0.51
1:C:574:THR:CG2	1:C:575:ASP:N	2.73	0.51
1:B:85:GLY:HA2	1:D:424:TYR:OH	2.10	0.51
1:B:560:PHE:CE1	1:C:559:CYS:HB3	2.45	0.51
1:D:145:SER:O	1:D:224:LYS:HD3	2.11	0.51
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.93	0.51
1:C:231:ALA:O	1:C:354:ASP:HA	2.11	0.51
1:B:80:TYR:HA	1:B:84:THR:HB	1.93	0.50
1:B:179:LEU:HD12	1:D:431:ILE:HD13	1.93	0.50
1:C:224:LYS:HE2	1:C:356:PRO:HD2	1.93	0.50
1:D:257:LEU:HB3	1:D:490:MET:HE1	1.94	0.50
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.94	0.50
1:B:231:ALA:HB1	1:B:371:PHE:CD2	2.46	0.50
1:D:29:VAL:HG12	1:D:141:THR:HG21	1.93	0.50
1:D:51:VAL:HG21	1:D:159:LEU:HD13	1.93	0.50
1:B:567:HIS:CE1	1:C:575:ASP:OD1	2.65	0.49
1:C:175:ALA:C	1:C:177:GLY:H	2.19	0.49
1:C:574:THR:CG2	1:C:575:ASP:H	2.25	0.49
1:D:524:THR:HG21	1:D:581:LEU:HD21	1.94	0.49
1:B:559:CYS:O	1:B:562:THR:HG22	2.12	0.49
1:B:559:CYS:HB3	1:C:560:PHE:CE1	2.47	0.49
1:D:374:SER:HA	1:D:463:SER:HB2	1.95	0.48
1:A:322:TYR:OH	1:B:176:SER:HB3	2.13	0.48
1:B:175:ALA:C	1:B:177:GLY:H	2.21	0.48
1:C:175:ALA:HB2	1:C:462:ASN:HB2	1.95	0.48
1:A:501:GLU:OE1	1:A:619:ARG:HD2	2.13	0.48
1:C:299:SER:HB3	1:C:302:GLN:HG2	1.94	0.48
1:A:524:THR:HG22	1:A:528:LEU:HD22	1.95	0.48
1:C:162:ASN:ND2	1:C:200:GLY:HA2	2.29	0.47
1:B:163:VAL:HG22	1:B:199:ILE:HG12	1.97	0.47
1:C:250:LEU:O	1:C:254:VAL:HG23	2.15	0.47
1:A:163:VAL:HG22	1:A:199:ILE:HG12	1.97	0.47
1:D:175:ALA:HB2	1:D:462:ASN:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:THR:HG23	1:D:562:THR:HG21	1.95	0.47
1:C:69:VAL:HG13	1:C:82:VAL:HG13	1.97	0.46
1:A:224:LYS:HE3	1:A:356:PRO:HD2	1.98	0.46
1:B:560:PHE:HB2	1:C:560:PHE:HB2	1.96	0.46
1:D:68:TRP:HE1	1:D:363:ASP:HA	1.79	0.46
1:C:80:TYR:CG	1:D:318:LYS:HG2	2.49	0.46
1:D:175:ALA:HB2	1:D:462:ASN:HB2	1.98	0.46
1:B:51:VAL:HG21	1:B:159:LEU:HD13	1.97	0.46
1:B:355:ASN:HB3	1:B:371:PHE:CE2	2.50	0.46
1:C:304:LEU:CD1	1:C:619:ARG:HD3	2.39	0.45
1:B:650:GLN:HG3	1:D:111:GLY:O	2.16	0.45
1:A:231:ALA:HB1	1:A:371:PHE:HD2	1.82	0.45
1:B:596:MET:O	1:B:599:VAL:HG12	2.16	0.45
1:A:353:ASN:HA	1:A:370:ASN:HB3	1.99	0.45
1:C:99:GLU:HA	1:C:102:GLU:CG	2.42	0.45
1:C:576:THR:HA	1:C:579:ASP:HB2	1.99	0.45
1:C:224:LYS:HG2	1:C:224:LYS:O	2.16	0.45
1:C:374:SER:HA	1:C:463:SER:HB2	1.99	0.45
1:C:145:SER:O	1:C:224:LYS:HD3	2.17	0.45
1:A:559:CYS:HB3	1:D:560:PHE:CE1	2.52	0.44
1:B:605:LYS:HB3	1:B:605:LYS:HE2	1.58	0.44
1:C:29:VAL:HG12	1:C:141:THR:HG21	1.99	0.44
1:B:175:ALA:HB2	1:B:462:ASN:CB	2.48	0.44
1:B:255:GLU:HG2	1:B:331:LEU:HD13	1.99	0.44
1:D:426:LEU:HG	1:D:429:LEU:HD12	1.99	0.44
1:B:81:GLY:HA3	1:B:227:LEU:HD22	1.99	0.44
1:A:355:ASN:HB3	1:A:371:PHE:CE2	2.53	0.44
1:D:380:MET:HE2	1:D:380:MET:HA	1.99	0.44
1:C:632:VAL:HA	1:C:636:LEU:HD12	2.00	0.44
1:D:181:PRO:HB2	1:D:235:PHE:CD2	2.52	0.44
1:B:345:VAL:O	1:B:349:VAL:HG23	2.17	0.43
1:A:567:HIS:CE1	1:D:579:ASP:OD1	2.71	0.43
1:D:501:GLU:OE1	1:D:619:ARG:HD2	2.18	0.43
1:B:175:ALA:HB2	1:B:462:ASN:HB2	1.98	0.43
1:D:79:ILE:HG22	1:D:82:VAL:HG13	2.01	0.43
1:A:299:SER:HA	1:A:300:PRO:HD2	1.87	0.43
1:A:374:SER:HA	1:A:463:SER:HB2	2.00	0.43
1:D:148:ARG:NH2	1:D:220:LYS:O	2.51	0.43
1:C:131:SER:HB3	1:C:238:ALA:HB1	2.00	0.43
1:C:380:MET:HA	1:C:380:MET:HE2	2.00	0.43
1:A:202:ASP:OD1	1:A:202:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ALA:O	1:B:354:ASP:HA	2.19	0.42
1:C:175:ALA:HB2	1:C:462:ASN:CB	2.49	0.42
1:B:72:LYS:HD3	1:B:72:LYS:HA	1.89	0.42
1:C:43:LEU:HD13	1:C:134:LEU:HD22	2.01	0.42
1:C:176:SER:HA	1:C:371:PHE:CD1	2.54	0.42
1:D:59:ARG:NH1	1:D:63:GLU:OE2	2.43	0.42
1:B:84:THR:HG22	1:B:85:GLY:O	2.20	0.42
1:A:512:SER:HB2	1:A:529:LEU:HD21	2.00	0.42
1:C:662:ASP:OD1	1:C:664:ARG:HD3	2.19	0.42
1:D:537:VAL:HA	1:D:540:TYR:CE2	2.54	0.42
1:A:27:ILE:CD1	1:A:43:LEU:HB2	2.49	0.42
1:A:588:LEU:HD12	1:A:588:LEU:HA	1.92	0.42
1:D:140:PHE:CG	1:D:147:ILE:HG21	2.54	0.42
1:D:318:LYS:O	1:D:318:LYS:HG3	2.19	0.42
1:B:59:ARG:HD2	1:B:63:GLU:CD	2.44	0.42
1:B:471:LYS:HA	1:B:471:LYS:HD3	1.84	0.42
1:B:540:TYR:CE1	1:B:551:LEU:HD22	2.55	0.42
1:C:265:ILE:O	1:C:266:PHE:HB2	2.19	0.42
1:B:66:SER:O	1:B:70:GLN:NE2	2.53	0.42
1:A:437:SER:O	1:A:441:GLN:HG2	2.20	0.41
1:C:224:LYS:NZ	1:C:354:ASP:OD2	2.54	0.41
1:C:21:PHE:O	1:C:46:ARG:NH1	2.53	0.41
1:D:178:ASP:HB3	1:D:181:PRO:HG2	2.03	0.41
1:D:631:PHE:O	1:D:635:GLU:HB2	2.21	0.41
1:B:662:ASP:OD1	1:B:664:ARG:HD3	2.21	0.41
1:D:27:ILE:CD1	1:D:43:LEU:HB2	2.51	0.41
1:A:299:SER:HB3	1:A:302:GLN:HG2	2.03	0.41
1:A:263:GLU:OE2	1:A:299:SER:OG	2.35	0.41
1:B:285:GLN:HB2	1:B:332:ALA:HB2	2.03	0.40
1:D:175:ALA:C	1:D:177:GLY:H	2.28	0.40
1:D:662:ASP:OD1	1:D:664:ARG:HD3	2.21	0.40
1:A:326:SER:HB3	1:B:369:ALA:CB	2.51	0.40
1:B:353:ASN:HA	1:B:370:ASN:HB3	2.04	0.40
1:B:26:LYS:HE2	1:B:52:ALA:HB2	2.04	0.40
1:C:99:GLU:HA	1:C:102:GLU:OE2	2.22	0.40
1:C:176:SER:OG	1:C:179:LEU:HD11	2.22	0.40
1:B:140:PHE:CG	1:B:147:ILE:HG21	2.57	0.40
1:B:499:LEU:HD21	1:B:600:ARG:HG3	2.03	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	612/707 (87%)	596 (97%)	16 (3%)	0	100	100
1	B	614/707 (87%)	592 (96%)	22 (4%)	0	100	100
1	C	613/707 (87%)	598 (98%)	15 (2%)	0	100	100
1	D	614/707 (87%)	597 (97%)	17 (3%)	0	100	100
All	All	2453/2828 (87%)	2383 (97%)	70 (3%)	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	527/592 (89%)	511 (97%)	16 (3%)	36	41
1	B	528/592 (89%)	512 (97%)	16 (3%)	36	41
1	C	528/592 (89%)	509 (96%)	19 (4%)	31	34
1	D	529/592 (89%)	510 (96%)	19 (4%)	31	34
All	All	2112/2368 (89%)	2042 (97%)	70 (3%)	33	37

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	71	ARG

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Mol	Chain	Res	Type
1	A	74	GLU
1	A	102	GLU
1	A	136	ARG
1	A	224	LYS
1	A	312	ASP
1	A	371	PHE
1	A	523	ASP
1	A	528	LEU
1	A	557	GLN
1	A	562	THR
1	A	567	HIS
1	A	575	ASP
1	A	583	GLU
1	A	619	ARG
1	B	43	LEU
1	B	59	ARG
1	B	70	GLN
1	B	75	ASP
1	B	99	GLU
1	B	102	GLU
1	B	107	CYS
1	B	209	GLU
1	B	212	SER
1	B	298	SER
1	B	312	ASP
1	B	371	PHE
1	B	528	LEU
1	B	605	LYS
1	B	624	LYS
1	B	670	LEU
1	C	23	GLU
1	C	59	ARG
1	C	106	ARG
1	C	107	CYS
1	C	135	LEU
1	C	136	ARG
1	C	212	SER
1	C	222	GLN
1	C	275	LEU
1	C	311	ILE
1	C	318	LYS
1	C	364	ARG

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Mol	Chain	Res	Type
1	C	371	PHE
1	C	528	LEU
1	C	542	GLU
1	C	562	THR
1	C	575	ASP
1	C	619	ARG
1	C	673	LEU
1	D	24	VAL
1	D	32	THR
1	D	43	LEU
1	D	59	ARG
1	D	82	VAL
1	D	100	LEU
1	D	107	CYS
1	D	136	ARG
1	D	162	ASN
1	D	227	LEU
1	D	371	PHE
1	D	455	GLU
1	D	528	LEU
1	D	562	THR
1	D	574	THR
1	D	575	ASP
1	D	605	LYS
1	D	635	GLU
1	D	673	LEU

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	22	ASN
1	A	222	GLN
1	A	462	ASN
1	A	557	GLN
1	A	567	HIS
1	B	22	ASN
1	B	70	GLN
1	B	362	ASN
1	B	456	GLN
1	B	462	ASN
1	B	557	GLN
1	C	22	ASN

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Mol	Chain	Res	Type
1	C	458	ASN
1	C	462	ASN
1	C	557	GLN
1	C	621	GLN
1	C	674	GLN
1	D	22	ASN
1	D	362	ASN
1	D	462	ASN
1	D	557	GLN
1	D	674	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2

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Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	78:ASP	C	79:ILE	N	1.10
1	B	78:ASP	C	79:ILE	N	1.05
1	D	78:ASP	C	79:ILE	N	1.03
1	B	77:ALA	C	78:ASP	N	0.91
1	A	77:ALA	C	78:ASP	N	0.90
1	D	77:ALA	C	78:ASP	N	0.88

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	624/707 (88%)	0.33	23 (3%) 45 47	27, 43, 66, 99	0
1	B	626/707 (88%)	0.42	26 (4%) 40 42	26, 45, 69, 91	0
1	C	625/707 (88%)	0.34	24 (3%) 44 46	27, 43, 68, 95	0
1	D	626/707 (88%)	0.37	21 (3%) 48 50	27, 43, 64, 81	0
All	All	2501/2828 (88%)	0.37	94 (3%) 44 46	26, 44, 67, 99	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	LEU	6.1
1	C	314	LEU	6.0
1	B	314	LEU	5.8
1	D	55	ALA	5.7
1	D	314	LEU	5.6
1	B	99	GLU	5.5
1	D	78	ASP	5.3
1	D	677	LEU	5.0
1	B	55	ALA	4.8
1	C	55	ALA	4.7
1	C	677	LEU	4.6
1	B	618	VAL	4.4
1	A	55	ALA	4.2
1	B	677	LEU	4.1
1	D	100	LEU	4.0
1	B	78	ASP	4.0
1	B	81	GLY	4.0
1	A	80	TYR	3.9
1	D	574	THR	3.9
1	A	78	ASP	3.8
1	A	100	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	82	VAL	3.7
1	C	99	GLU	3.7
1	B	578	VAL	3.5
1	C	313	LYS	3.4
1	B	86	PHE	3.4
1	C	82	VAL	3.4
1	B	84	THR	3.2
1	C	315	LYS	3.1
1	C	575	ASP	3.1
1	A	361	ALA	3.0
1	C	566	LEU	3.0
1	C	80	TYR	3.0
1	C	318	LYS	3.0
1	A	79	ILE	2.9
1	B	313	LYS	2.9
1	B	79	ILE	2.9
1	D	575	ASP	2.9
1	B	77	ALA	2.9
1	C	76	GLY	2.8
1	B	83	THR	2.8
1	B	581	LEU	2.8
1	B	70	GLN	2.7
1	D	82	VAL	2.7
1	C	114	THR	2.7
1	A	602	LEU	2.6
1	B	100	LEU	2.6
1	B	311	ILE	2.6
1	D	79	ILE	2.6
1	D	364	ARG	2.6
1	C	589	SER	2.6
1	B	80	TYR	2.6
1	A	75	ASP	2.6
1	C	58	CYS	2.6
1	A	574	THR	2.5
1	D	83	THR	2.5
1	C	523	ASP	2.5
1	B	85	GLY	2.5
1	B	122	ASP	2.5
1	A	222	GLN	2.5
1	B	315	LYS	2.5
1	D	315	LYS	2.4
1	C	312	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	71	ARG	2.4
1	A	81	GLY	2.4
1	B	605	LYS	2.3
1	A	618	VAL	2.3
1	C	67	SER	2.3
1	A	545	CYS	2.3
1	C	100	LEU	2.3
1	A	223	ALA	2.3
1	A	314	LEU	2.3
1	A	605	LYS	2.2
1	D	102	GLU	2.2
1	D	298	SER	2.2
1	D	587	ARG	2.2
1	D	69	VAL	2.2
1	C	564	LEU	2.2
1	B	584	PHE	2.2
1	D	122	ASP	2.2
1	C	51	VAL	2.2
1	C	79	ILE	2.1
1	C	574	THR	2.1
1	C	106	ARG	2.1
1	A	25	LYS	2.1
1	D	576	THR	2.1
1	A	567	HIS	2.1
1	A	77	ALA	2.1
1	D	51	VAL	2.1
1	A	575	ASP	2.0
1	A	590	ASP	2.0
1	D	567	HIS	2.0
1	D	618	VAL	2.0
1	B	58	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.