



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:49 PM UTC

PDB ID : 3RBL / pdb_00003rbl
Title : Crystal structure of Human aromatic L-amino acid decarboxylase (AADC) in the apo form
Authors : Giardina, G.; Montioli, R.; Gianni, S.; Cellini, B.; Paiardini, A.; Borri Voltattorni, C.; Cutruzzola, F.
Deposited on : 2011-03-29
Resolution : 3.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

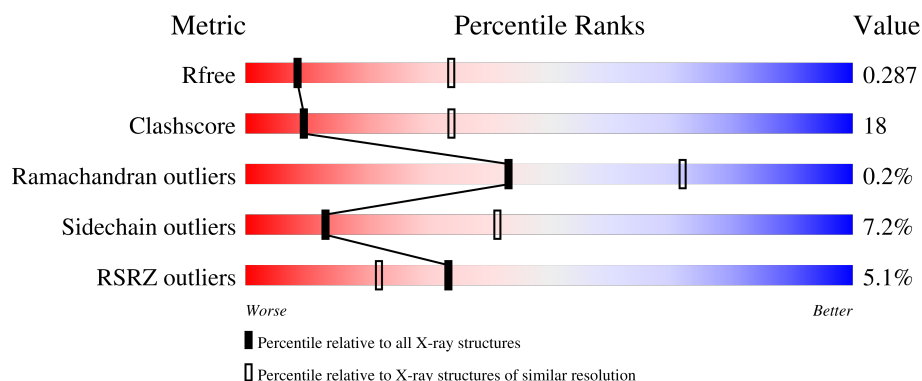
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	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	480	
1	B	480	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6950 atoms, of which 0 are hydrogens and 0 are deuteriums.

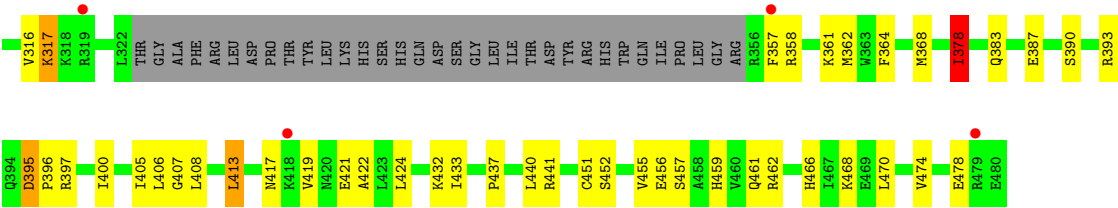
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called aromatic L-amino acid decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3469	2221	599	622	27			
1	B	443	Total	C	N	O	S	0	0	0
			3480	2229	601	624	26			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.64Å 179.64Å 74.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.24 30.00 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-3.24) 99.2 (30.00-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.294 0.238 , 0.287	Depositor DCC
R_{free} test set	1024 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 20.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6950	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.69	0/3548	0.96	8/4798 (0.2%)
1	B	0.73	0/3561	1.02	11/4817 (0.2%)
All	All	0.71	0/7109	0.99	19/9615 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	THR	N-CA-C	7.54	119.50	111.28
1	A	195	VAL	CA-C-N	6.57	129.38	120.38
1	A	195	VAL	C-N-CA	6.57	129.38	120.38
1	B	407	GLY	N-CA-C	6.57	120.84	112.83
1	A	441	ARG	CB-CA-C	-6.41	109.17	116.54
1	A	100	CYS	N-CA-C	5.98	118.19	108.26
1	B	441	ARG	CB-CA-C	-5.95	109.73	116.63
1	A	442	ASP	N-CA-C	5.75	117.62	111.36
1	B	395	ASP	CA-C-N	5.59	126.65	120.45
1	B	395	ASP	C-N-CA	5.59	126.65	120.45
1	B	108	SER	CA-C-N	5.51	124.71	118.97
1	B	108	SER	C-N-CA	5.51	124.71	118.97
1	B	378	ILE	CB-CA-C	-5.38	104.88	112.14
1	B	239	MET	N-CA-C	5.33	117.18	108.55
1	A	295	ASP	N-CA-C	-5.22	107.46	113.88
1	A	34	GLU	CA-C-N	5.21	126.36	119.84
1	A	34	GLU	C-N-CA	5.21	126.36	119.84
1	B	42	ILE	CA-C-N	5.00	126.10	119.84
1	B	42	ILE	C-N-CA	5.00	126.10	119.84

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	3469	0	3456	146	0
1	B	3480	0	3466	108	0
2	B	1	0	0	0	0
All	All	6950	0	6922	244	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 18.

All (244) 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:124:LYS:HE3	1:A:135:GLU:OE1	1.36	1.23
1:A:432:LYS:HD3	1:A:466:HIS:CG	1.79	1.18
1:A:116:THR:CG2	1:A:134:ASN:HD21	1.64	1.10
1:A:452:SER:OG	1:A:455:VAL:HG23	1.51	1.08
1:A:124:LYS:CE	1:A:135:GLU:OE1	2.01	1.07
1:A:116:THR:HG22	1:A:134:ASN:ND2	1.71	1.06
1:A:116:THR:HG22	1:A:134:ASN:HD21	0.89	1.05
1:A:80:PHE:CE2	1:A:451:CYS:O	2.12	1.03
1:A:120:ASP:OD2	1:A:134:ASN:OD1	1.79	1.01
1:A:53:PHE:CE2	1:A:57:ILE:HD11	1.97	1.00
1:A:456:GLU:H	1:A:459:HIS:HD2	1.05	0.99
1:A:30:TYR:OH	1:A:434:HIS:CD2	2.16	0.98
1:A:302:HIS:HB3	1:A:311:CYS:HB3	1.43	0.97
1:A:116:THR:CG2	1:A:134:ASN:ND2	2.26	0.96
1:A:432:LYS:HB3	1:A:466:HIS:CE1	2.02	0.94
1:B:304:TRP:HB3	1:B:378:ILE:CD1	1.99	0.92
1:B:456:GLU:H	1:B:459:HIS:HD2	1.13	0.91
1:B:274:TYR:HE1	1:B:300:ASN:HD22	0.99	0.90
1:A:217:MET:SD	1:A:239:MET:HE1	2.14	0.88
1:A:83:ALA:HB3	1:A:302:HIS:O	1.75	0.86
1:A:456:GLU:H	1:A:459:HIS:CD2	1.94	0.86
1:B:189:ASP:OD2	1:B:211:SER:OG	1.94	0.85
1:A:80:PHE:H	1:A:80:PHE:HD2	1.25	0.84
1:A:131:ALA:O	1:A:140:GLY:HA3	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:HIS:ND1	1:A:311:CYS:O	2.11	0.83
1:B:387:GLU:OE2	1:B:457:SER:HB2	1.81	0.81
1:B:302:HIS:HD2	1:B:307:VAL:O	1.64	0.80
1:A:432:LYS:HD3	1:A:466:HIS:CD2	2.16	0.79
1:A:30:TYR:HH	1:A:434:HIS:CD2	2.00	0.79
1:A:99:GLY:HA3	1:B:80:PHE:HZ	1.48	0.78
1:A:124:LYS:HE3	1:A:135:GLU:CD	2.09	0.78
1:A:288:LEU:O	1:A:291:VAL:HG23	1.84	0.78
1:A:98:ILE:HG21	1:B:68:VAL:HG21	1.66	0.77
1:B:432:LYS:HE2	1:B:462:ARG:NH1	2.00	0.77
1:B:53:PHE:CE2	1:B:57:ILE:HD11	2.20	0.77
1:B:304:TRP:HB3	1:B:378:ILE:HD13	1.65	0.77
1:B:29:VAL:O	1:B:69:THR:O	2.05	0.75
1:A:456:GLU:N	1:A:459:HIS:HD2	1.83	0.74
1:B:307:VAL:HG12	1:B:308:ASN:N	2.02	0.74
1:B:180:MET:HA	1:B:183:LEU:HD22	1.69	0.73
1:A:307:VAL:HG11	1:A:311:CYS:SG	2.29	0.73
1:B:307:VAL:CG1	1:B:308:ASN:N	2.51	0.72
1:B:212:ASP:C	1:B:212:ASP:OD1	2.30	0.72
1:A:144:ILE:HG23	1:A:312:SER:O	1.90	0.72
1:A:136:LYS:O	1:A:137:ALA:HB3	1.87	0.72
1:B:249:CYS:SG	1:B:406:LEU:HD12	2.30	0.72
1:A:432:LYS:HD3	1:A:466:HIS:ND1	2.05	0.72
1:B:239:MET:CE	1:B:261:CYS:SG	2.78	0.72
1:A:192:HIS:HD2	1:A:194:SER:HB3	1.56	0.71
1:B:245:THR:O	1:B:248:CYS:O	2.08	0.71
1:B:424:LEU:HD22	1:B:437:PRO:HG3	1.72	0.70
1:A:124:LYS:NZ	1:A:135:GLU:OE1	2.26	0.69
1:B:239:MET:HE2	1:B:261:CYS:SG	2.33	0.69
1:B:456:GLU:N	1:B:459:HIS:HD2	1.90	0.68
1:A:218:ARG:NH1	1:A:256:GLU:OE2	2.26	0.68
1:A:101:ILE:HB	1:B:82:THR:HG21	1.74	0.67
1:A:302:HIS:ND1	1:A:309:PHE:O	2.26	0.67
1:B:211:SER:HB2	1:B:215:PHE:HA	1.74	0.67
1:B:274:TYR:HE1	1:B:300:ASN:ND2	1.84	0.67
1:B:196:GLU:HA	1:B:206:LEU:HD22	1.76	0.66
1:B:222:LEU:O	1:B:226:LEU:HG	1.95	0.66
1:A:120:ASP:CG	1:A:134:ASN:OD1	2.40	0.65
1:A:429:SER:O	1:A:431:LYS:HG2	1.97	0.64
1:B:456:GLU:H	1:B:459:HIS:CD2	2.06	0.64
1:B:196:GLU:HA	1:B:206:LEU:CD2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:HB3	1:A:63:ILE:HD12	1.80	0.64
1:B:452:SER:OG	1:B:455:VAL:CG2	2.47	0.63
1:A:94:LEU:HD23	1:A:360:LEU:HD21	1.80	0.62
1:B:466:HIS:CE1	1:B:470:LEU:HD11	2.33	0.62
1:A:395:ASP:OD1	1:A:396:PRO:HD2	1.99	0.62
1:B:189:ASP:CG	1:B:211:SER:OG	2.43	0.62
1:A:10:GLY:O	1:A:14:VAL:HG23	2.00	0.62
1:A:413:LEU:HD22	1:A:423:LEU:HD22	1.82	0.62
1:B:452:SER:OG	1:B:455:VAL:HG23	1.99	0.61
1:A:192:HIS:CD2	1:A:194:SER:H	2.16	0.61
1:A:98:ILE:CG2	1:B:68:VAL:HG21	2.29	0.61
1:A:136:LYS:O	1:A:137:ALA:CB	2.48	0.61
1:B:189:ASP:CG	1:B:211:SER:HG	2.08	0.61
1:A:53:PHE:CD2	1:A:57:ILE:HD11	2.36	0.61
1:A:452:SER:CB	1:A:455:VAL:HG23	2.31	0.61
1:A:192:HIS:HD2	1:A:194:SER:H	1.48	0.61
1:A:389:GLU:OE2	1:A:393:ARG:NH2	2.34	0.61
1:A:192:HIS:CD2	1:A:194:SER:HB3	2.36	0.60
1:B:122:LEU:HA	1:B:125:MET:HE3	1.83	0.60
1:B:303:LYS:HE3	1:B:451:CYS:SG	2.42	0.59
1:A:452:SER:OG	1:A:455:VAL:CG2	2.41	0.59
1:A:288:LEU:HG	1:A:291:VAL:HG21	1.85	0.59
1:A:357:PHE:CD1	1:A:360:LEU:HB2	2.38	0.59
1:A:1:MET:HE3	1:B:87:PRO:HG3	1.83	0.59
1:A:424:LEU:HD22	1:A:437:PRO:HG3	1.84	0.59
1:A:150:GLU:O	1:A:154:VAL:HG23	2.02	0.58
1:B:302:HIS:CD2	1:B:307:VAL:O	2.52	0.58
1:B:424:LEU:CD2	1:B:437:PRO:HG3	2.34	0.58
1:A:363:TRP:O	1:A:367:ARG:HG3	2.04	0.57
1:A:85:SER:O	1:A:89:MET:HG3	2.04	0.57
1:B:212:ASP:OD1	1:B:214:ASN:N	2.37	0.57
1:B:277:SER:CB	1:B:304:TRP:HB2	2.35	0.56
1:B:71:TRP:H	1:B:71:TRP:CD1	2.23	0.56
1:A:392:VAL:HG22	1:A:464:TRP:CZ3	2.42	0.55
1:A:1:MET:HE1	1:B:368:MET:SD	2.46	0.55
1:A:288:LEU:HG	1:A:291:VAL:CG2	2.36	0.55
1:A:294:ALA:O	1:A:317:LYS:HE2	2.07	0.55
1:B:288:LEU:O	1:B:288:LEU:HG	2.07	0.55
1:A:6:PHE:O	1:A:10:GLY:N	2.38	0.54
1:A:145:GLN:O	1:A:312:SER:HB3	2.08	0.54
1:A:364:PHE:O	1:A:368:MET:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LEU:HB3	1:B:294:ALA:HA	1.90	0.54
1:A:432:LYS:CD	1:A:466:HIS:CG	2.73	0.54
1:B:254:LEU:HB3	1:B:290:GLY:HA3	1.90	0.54
1:A:30:TYR:CE2	1:A:434:HIS:CG	2.96	0.53
1:A:466:HIS:O	1:A:470:LEU:HG	2.08	0.53
1:A:300:ASN:HB2	1:A:303:LYS:HG3	1.91	0.53
1:B:65:MET:O	1:B:68:VAL:HG12	2.09	0.53
1:A:100:CYS:HG	1:A:357:PHE:HD2	1.54	0.53
1:A:307:VAL:CG1	1:A:311:CYS:HB2	2.39	0.53
1:B:364:PHE:CD2	1:B:368:MET:CE	2.92	0.53
1:A:432:LYS:CD	1:A:466:HIS:CD2	2.90	0.53
1:B:1:MET:HE3	1:B:5:GLU:HB3	1.91	0.53
1:B:126:LEU:HD11	1:B:299:PHE:CE2	2.43	0.53
1:A:79:TYR:HA	1:A:451:CYS:SG	2.49	0.53
1:A:52:THR:HG22	1:A:54:GLU:OE1	2.10	0.52
1:A:357:PHE:CE1	1:A:360:LEU:HB2	2.44	0.52
1:B:134:ASN:OD1	1:B:142:GLY:N	2.18	0.52
1:A:33:VAL:HG11	1:A:37:TYR:CG	2.45	0.52
1:A:80:PHE:CZ	1:A:451:CYS:O	2.59	0.52
1:A:98:ILE:O	1:A:99:GLY:C	2.53	0.52
1:B:308:ASN:HB3	1:B:361:LYS:HD2	1.92	0.52
1:A:430:ALA:O	1:A:431:LYS:HB2	2.09	0.52
1:A:399:GLU:OE2	1:A:412:ARG:HD3	2.10	0.52
1:B:85:SER:O	1:B:89:MET:HG3	2.10	0.52
1:B:164:ILE:HG12	1:B:179:ILE:HG21	1.91	0.51
1:A:7:ARG:O	1:A:11:LYS:HG3	2.09	0.51
1:A:79:TYR:CZ	1:A:81:PRO:HA	2.46	0.51
1:B:277:SER:HB2	1:B:304:TRP:HB2	1.92	0.51
1:A:406:LEU:O	1:A:406:LEU:HG	2.10	0.51
1:A:426:ARG:HB3	1:A:470:LEU:HD13	1.92	0.51
1:B:245:THR:OG1	1:B:250:SER:HB3	2.10	0.51
1:B:364:PHE:CD2	1:B:368:MET:HE1	2.46	0.50
1:A:228:ARG:HD2	1:A:229:ASP:OD1	2.11	0.50
1:B:57:ILE:O	1:B:60:VAL:HB	2.11	0.50
1:B:19:ASN:O	1:B:20:TYR:C	2.53	0.50
1:B:307:VAL:CG1	1:B:308:ASN:H	2.20	0.50
1:A:384:LEU:HD22	1:A:457:SER:HA	1.94	0.50
1:B:75:TYR:HB3	1:B:433:ILE:HG22	1.94	0.50
1:A:397:ARG:O	1:A:413:LEU:HD12	2.12	0.50
1:B:1:MET:HB2	1:B:5:GLU:OE1	2.12	0.50
1:A:239:MET:HG2	1:A:261:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LYS:O	1:A:365:VAL:HG23	2.12	0.50
1:B:432:LYS:HE2	1:B:462:ARG:HH12	1.74	0.49
1:A:364:PHE:CD2	1:A:368:MET:HE3	2.47	0.49
1:A:382:VAL:O	1:A:385:SER:HB3	2.12	0.49
1:B:238:PHE:CD2	1:B:267:TRP:CD1	3.01	0.49
1:A:99:GLY:HA3	1:B:80:PHE:CZ	2.39	0.49
1:B:95:CYS:SG	1:B:357:PHE:HB2	2.53	0.48
1:B:419:VAL:O	1:B:422:ALA:HB3	2.13	0.48
1:A:30:TYR:HE2	1:A:434:HIS:CB	2.27	0.48
1:B:457:SER:O	1:B:461:GLN:HG2	2.14	0.48
1:A:398:PHE:O	1:A:414:LYS:HE3	2.14	0.48
1:B:12:GLU:O	1:B:15:ASP:HB2	2.14	0.47
1:A:71:TRP:HD1	1:A:76:PHE:CE2	2.31	0.47
1:B:262:ASN:ND2	1:B:293:PHE:HD1	2.12	0.47
1:B:294:ALA:O	1:B:317:LYS:HE2	2.14	0.47
1:B:53:PHE:CZ	1:B:57:ILE:HD11	2.49	0.47
1:B:307:VAL:HG13	1:B:308:ASN:H	1.79	0.47
1:B:309:PHE:C	1:B:311:CYS:H	2.22	0.47
1:A:408:LEU:HD11	1:A:447:ARG:HB3	1.97	0.47
1:A:38:LEU:CD1	1:A:63:ILE:HG22	2.45	0.47
1:B:117:VAL:HG12	1:B:118:MET:HE2	1.97	0.46
1:A:306:LEU:HD21	1:A:377:TYR:CZ	2.49	0.46
1:A:432:LYS:HD3	1:A:466:HIS:CE1	2.50	0.46
1:A:175:THR:HG23	1:A:178:ALA:H	1.79	0.46
1:B:361:LYS:O	1:B:362:MET:C	2.59	0.46
1:A:435:LEU:HG	1:A:447:ARG:O	2.16	0.46
1:A:302:HIS:CE1	1:A:311:CYS:O	2.68	0.46
1:A:42:ILE:HG21	1:B:117:VAL:HG11	1.97	0.45
1:B:272:ALA:HB3	1:B:299:PHE:HB3	1.98	0.45
1:B:387:GLU:O	1:B:390:SER:HB2	2.16	0.45
1:A:30:TYR:HE2	1:A:434:HIS:CG	2.33	0.45
1:A:277:SER:HB3	1:A:305:LEU:HG	1.98	0.45
1:A:272:ALA:O	1:A:273:ALA:C	2.59	0.45
1:A:274:TYR:HA	1:A:303:LYS:HD2	1.98	0.45
1:B:20:TYR:CZ	1:B:24:ILE:HD12	2.52	0.45
1:A:1:MET:HE2	1:A:1:MET:HB3	1.89	0.44
1:A:302:HIS:HB2	1:A:309:PHE:HA	1.99	0.44
1:A:440:LEU:O	1:A:441:ARG:C	2.59	0.44
1:B:228:ARG:HD2	1:B:229:ASP:OD1	2.17	0.44
1:B:277:SER:O	1:B:280:ILE:HG12	2.17	0.44
1:B:310:ASP:CG	1:B:358:ARG:HD3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.75	0.44
1:B:397:ARG:O	1:B:413:LEU:HD12	2.18	0.44
1:A:196:GLU:HA	1:A:206:LEU:HD22	2.00	0.43
1:B:197:ARG:HE	1:B:201:ILE:HD11	1.83	0.43
1:B:212:ASP:OD1	1:B:213:GLY:N	2.51	0.43
1:A:211:SER:HB2	1:A:215:PHE:HA	2.01	0.43
1:B:364:PHE:HD2	1:B:368:MET:HE1	1.83	0.43
1:A:200:LEU:N	1:A:200:LEU:CD1	2.82	0.43
1:B:224:GLU:O	1:B:225:ALA:C	2.61	0.43
1:B:1:MET:CE	1:B:5:GLU:HB3	2.47	0.43
1:A:305:LEU:O	1:A:306:LEU:HB2	2.18	0.43
1:A:133:LEU:HD23	1:A:135:GLU:OE2	2.19	0.42
1:B:417:ASN:O	1:B:421:GLU:HG3	2.19	0.42
1:A:19:ASN:O	1:A:20:TYR:C	2.62	0.42
1:A:307:VAL:HG12	1:A:311:CYS:HB2	2.01	0.42
1:A:288:LEU:CG	1:A:291:VAL:HG21	2.49	0.42
1:A:307:VAL:HG11	1:A:311:CYS:HB2	2.01	0.42
1:B:395:ASP:HA	1:B:396:PRO:HD3	1.70	0.42
1:A:34:GLU:HA	1:A:35:PRO:HD2	1.74	0.42
1:A:119:MET:HE1	1:A:313:ALA:HB1	2.02	0.42
1:A:281:CYS:HA	1:A:282:PRO:HD3	1.95	0.42
1:A:75:TYR:HA	1:A:77:PHE:CE1	2.54	0.42
1:A:100:CYS:SG	1:A:357:PHE:HD2	2.42	0.42
1:B:30:TYR:HD2	1:B:31:PRO:HD2	1.84	0.42
1:B:68:VAL:CG1	1:B:70:HIS:CE1	3.02	0.42
1:B:80:PHE:CD2	1:B:83:ALA:HB2	2.55	0.41
1:A:33:VAL:HG11	1:A:37:TYR:CD1	2.55	0.41
1:A:468:LYS:O	1:A:469:GLU:C	2.63	0.41
1:A:68:VAL:HG11	1:B:98:ILE:HG23	2.02	0.41
1:B:308:ASN:OD1	1:B:310:ASP:HB3	2.20	0.41
1:A:100:CYS:O	1:A:101:ILE:HG13	2.21	0.41
1:A:307:VAL:HG11	1:A:311:CYS:CB	2.51	0.41
1:B:238:PHE:CE2	1:B:267:TRP:CD1	3.09	0.41
1:B:303:LYS:HE2	1:B:304:TRP:CZ2	2.55	0.41
1:A:180:MET:HE3	1:A:180:MET:HB3	1.72	0.41
1:B:310:ASP:OD2	1:B:358:ARG:HD3	2.20	0.41
1:A:4:SER:O	1:A:7:ARG:HB2	2.20	0.41
1:A:27:ARG:HH12	1:A:65:MET:HB3	1.85	0.41
1:A:82:THR:HA	1:A:309:PHE:HB3	2.03	0.41
1:A:275:ALA:HB1	1:A:406:LEU:HD11	2.02	0.41
1:A:56:ILE:O	1:A:60:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:TYR:CD1	1:A:274:TYR:C	2.98	0.41
1:B:160:ARG:O	1:B:163:VAL:HG12	2.21	0.41
1:B:219:ALA:HB2	1:B:256:GLU:HB3	2.02	0.41
1:A:190:GLN:NE2	1:A:215:PHE:HD2	2.19	0.40
1:A:262:ASN:ND2	1:A:293:PHE:HD1	2.19	0.40
1:B:30:TYR:CD2	1:B:31:PRO:HD2	2.56	0.40
1:A:13:MET:HE2	1:A:53:PHE:HZ	1.86	0.40
1:A:38:LEU:O	1:A:39:ARG:C	2.65	0.40
1:A:60:VAL:HG11	1:B:94:LEU:HD21	2.04	0.40
1:A:83:ALA:CB	1:A:302:HIS:O	2.59	0.40
1:B:238:PHE:HD2	1:B:267:TRP:CD1	2.38	0.40
1:A:80:PHE:HA	1:A:81:PRO:HD2	1.94	0.40
1:B:91:ALA:HB3	1:B:361:LYS:HG2	2.04	0.40
1:A:394:GLN:NE2	1:A:394:GLN:HA	2.35	0.40
1:B:125:MET:HB3	1:B:280:ILE:HG22	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	436/480 (91%)	398 (91%)	36 (8%)	2 (0%)	24	56
1	B	437/480 (91%)	413 (94%)	24 (6%)	0	100	100
All	All	873/960 (91%)	811 (93%)	60 (7%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	SER
1	A	427	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	366/399 (92%)	345 (94%)	21 (6%)	18	49
1	B	366/399 (92%)	334 (91%)	32 (9%)	9	33
All	All	732/798 (92%)	679 (93%)	53 (7%)	13	41

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	80	PHE
1	A	82	THR
1	A	101	ILE
1	A	116	THR
1	A	167	LEU
1	A	174	LEU
1	A	184	VAL
1	A	196	GLU
1	A	220	SER
1	A	265	ASP
1	A	277	SER
1	A	283	GLU
1	A	318	LYS
1	A	394	GLN
1	A	400	ILE
1	A	413	LEU
1	A	418	LYS
1	A	435	LEU
1	A	443	LYS
1	A	476	ARG
1	B	17	VAL
1	B	71	TRP
1	B	73	SER
1	B	92	ASP
1	B	133	LEU
1	B	139	GLU

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Mol	Chain	Res	Type
1	B	145	GLN
1	B	167	LEU
1	B	181	GLU
1	B	183	LEU
1	B	211	SER
1	B	214	ASN
1	B	220	SER
1	B	230	LYS
1	B	243	LEU
1	B	246	THR
1	B	249	CYS
1	B	254	LEU
1	B	291	VAL
1	B	316	VAL
1	B	317	LYS
1	B	378	ILE
1	B	383	GLN
1	B	393	ARG
1	B	400	ILE
1	B	405	ILE
1	B	408	LEU
1	B	413	LEU
1	B	440	LEU
1	B	468	LYS
1	B	474	VAL
1	B	478	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	176	GLN
1	A	192	HIS
1	A	262	ASN
1	A	375	GLN
1	A	394	GLN
1	A	434	HIS
1	A	459	HIS
1	A	466	HIS
1	B	145	GLN
1	B	308	ASN
1	B	459	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	442/480 (92%)	0.38	29 (6%) 24 16	23, 47, 58, 69	8 (1%)
1	B	443/480 (92%)	0.21	16 (3%) 46 29	25, 44, 57, 68	8 (1%)
All	All	885/960 (92%)	0.29	45 (5%) 33 22	23, 45, 58, 69	16 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	ARG	11.3
1	A	319	ARG	9.5
1	B	357	PHE	8.6
1	A	136	LYS	8.1
1	B	136	LYS	7.4
1	A	311	CYS	6.7
1	A	9	ARG	6.7
1	A	465	GLU	6.6
1	A	130	LYS	5.3
1	A	71	TRP	4.9
1	B	230	LYS	4.5
1	A	310	ASP	4.5
1	B	107	ALA	4.3
1	B	173	GLU	3.9
1	A	138	GLY	3.7
1	B	106	ALA	3.5
1	A	80	PHE	3.3
1	A	139	GLU	3.3
1	B	319	ARG	3.3
1	A	451	CYS	3.2
1	A	137	ALA	3.2
1	B	479	ARG	3.1
1	A	192	HIS	3.1
1	A	194	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	418	LYS	2.9
1	A	135	GLU	2.8
1	A	79	TYR	2.7
1	A	193	SER	2.6
1	B	134	ASN	2.6
1	B	133	LEU	2.6
1	B	137	ALA	2.6
1	B	105	TRP	2.6
1	A	99	GLY	2.6
1	A	112	THR	2.5
1	A	81	PRO	2.5
1	A	140	GLY	2.4
1	A	432	LYS	2.3
1	B	104	SER	2.3
1	B	108	SER	2.2
1	A	30	TYR	2.1
1	A	477	ALA	2.1
1	A	83	ALA	2.1
1	A	479	ARG	2.0
1	A	101	ILE	2.0
1	B	308	ASN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	481	1/1	0.96	0.07	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.