



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:15 PM UTC

PDB ID : 2CY8 / pdb_00002cy8
Title : Crystal structure of D-phenylglycine aminotransferase (D-PhgAT) from *Pseudomonas strutzeri* ST-201
Authors : Kongsaree, P.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-05
Resolution : 2.30 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

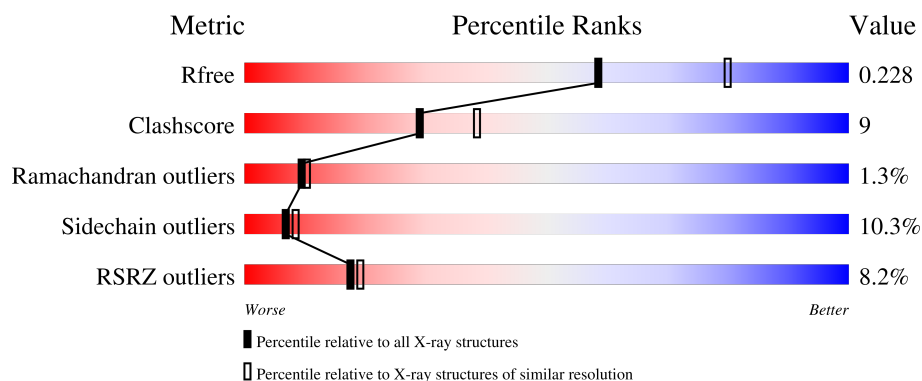
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	453	7% 53% 28% 5% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3185 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 D-phenylglycine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3055	1926	555	562	12			

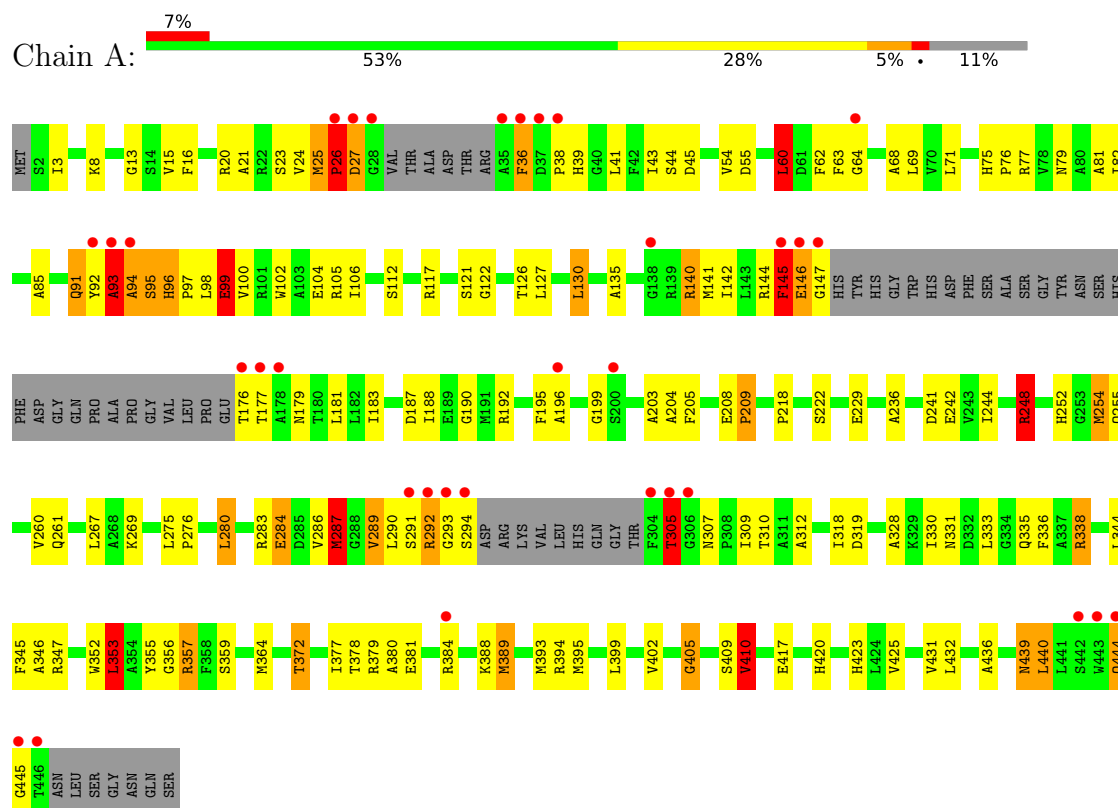
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	130	Total	O	0	0
			130	130		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: D-phenylglycine aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	74.68Å 74.68Å 147.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.60 – 2.30 31.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (31.60-2.30) 95.4 (31.60-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.27 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.184 , 0.223 0.191 , 0.228	Depositor DCC
R_{free} test set	1073 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3185	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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	2.16	105/3116 (3.4%)	1.60	32/4216 (0.8%)

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	MET	SD-CE	9.21	2.02	1.79
1	A	75	HIS	CA-C	9.06	1.62	1.53
1	A	94	ALA	CA-CB	8.51	1.66	1.53
1	A	69	LEU	CA-C	-8.20	1.44	1.53
1	A	145	PHE	CB-CG	-8.20	1.31	1.50
1	A	100	VAL	CA-CB	7.99	1.64	1.54
1	A	318	ILE	CA-CB	-7.79	1.45	1.54
1	A	44	SER	C-O	-7.54	1.14	1.24
1	A	312	ALA	CA-CB	-7.45	1.41	1.53
1	A	45	ASP	CA-C	-7.42	1.43	1.52
1	A	8	LYS	C-O	-7.38	1.15	1.24
1	A	79	ASN	C-O	-7.34	1.15	1.24
1	A	328	ALA	CA-CB	7.33	1.65	1.53
1	A	410	VAL	N-CA	-7.25	1.37	1.46
1	A	439	ASN	CB-CG	-7.23	1.33	1.52
1	A	440	LEU	C-O	-7.16	1.14	1.23
1	A	92	TYR	CA-C	7.06	1.60	1.52
1	A	76	PRO	C-O	-6.86	1.16	1.24
1	A	93	ALA	N-CA	6.63	1.54	1.46
1	A	102	TRP	C-O	-6.63	1.16	1.24
1	A	190	GLY	CA-C	6.63	1.60	1.52
1	A	345	PHE	C-O	-6.61	1.16	1.24
1	A	252	HIS	CA-CB	6.61	1.63	1.53
1	A	431	VAL	C-O	-6.51	1.16	1.24
1	A	94	ALA	N-CA	6.50	1.54	1.46
1	A	336	PHE	N-CA	-6.48	1.38	1.46
1	A	380	ALA	C-O	-6.47	1.15	1.23
1	A	410	VAL	CB-CG2	-6.46	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	MET	N-CA	6.44	1.54	1.46
1	A	21	ALA	CA-C	-6.42	1.44	1.52
1	A	284	GLU	CA-C	-6.41	1.44	1.52
1	A	82	ILE	CA-CB	-6.39	1.46	1.54
1	A	353	LEU	CG-CD1	-6.34	1.31	1.52
1	A	394	ARG	N-CA	-6.29	1.38	1.46
1	A	95	SER	N-CA	-6.28	1.38	1.46
1	A	289	VAL	C-O	-6.24	1.16	1.24
1	A	39	HIS	CA-CB	6.24	1.64	1.53
1	A	36	PHE	CA-C	6.21	1.60	1.52
1	A	16	PHE	CA-C	6.14	1.60	1.52
1	A	267	LEU	C-O	6.14	1.31	1.23
1	A	203	ALA	CA-CB	6.12	1.63	1.53
1	A	389	MET	CA-C	6.09	1.60	1.52
1	A	92	TYR	C-O	6.08	1.32	1.23
1	A	106	ILE	N-CA	-6.05	1.39	1.46
1	A	64	GLY	CA-C	6.03	1.60	1.51
1	A	192	ARG	C-O	5.95	1.31	1.24
1	A	377	ILE	CA-CB	5.86	1.62	1.54
1	A	140	ARG	CA-C	5.85	1.59	1.52
1	A	3	ILE	N-CA	5.84	1.53	1.46
1	A	432	LEU	N-CA	-5.84	1.39	1.46
1	A	388	LYS	C-O	-5.83	1.17	1.24
1	A	248	ARG	NE-CZ	5.82	1.39	1.33
1	A	204	ALA	N-CA	5.81	1.53	1.45
1	A	43	ILE	N-CA	-5.80	1.39	1.46
1	A	122	GLY	CA-C	-5.77	1.45	1.52
1	A	405	GLY	C-O	5.76	1.31	1.23
1	A	96	HIS	CA-C	5.74	1.59	1.53
1	A	85	ALA	CA-CB	-5.68	1.44	1.53
1	A	13	GLY	CA-C	5.65	1.58	1.52
1	A	99	GLU	CA-C	5.65	1.60	1.52
1	A	305	THR	C-O	-5.65	1.16	1.24
1	A	187	ASP	C-O	-5.61	1.17	1.23
1	A	24	VAL	CA-CB	-5.60	1.48	1.54
1	A	402	VAL	CB-CG1	-5.60	1.34	1.52
1	A	85	ALA	CA-C	-5.60	1.45	1.52
1	A	269	LYS	C-O	-5.59	1.17	1.24
1	A	54	VAL	C-O	-5.53	1.16	1.24
1	A	82	ILE	C-O	-5.52	1.17	1.24
1	A	145	PHE	CA-C	-5.51	1.45	1.53
1	A	445	GLY	C-O	5.50	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	ALA	CA-C	-5.47	1.45	1.52
1	A	81	ALA	CA-CB	-5.47	1.44	1.53
1	A	252	HIS	CA-C	-5.45	1.46	1.52
1	A	254	MET	N-CA	-5.44	1.39	1.46
1	A	229	GLU	N-CA	5.42	1.52	1.46
1	A	236	ALA	CA-CB	-5.40	1.45	1.53
1	A	208	GLU	CD-OE1	5.39	1.35	1.25
1	A	444	GLN	CA-C	5.39	1.59	1.52
1	A	432	LEU	CA-C	5.37	1.59	1.52
1	A	393	MET	C-O	-5.34	1.18	1.24
1	A	399	LEU	CA-C	-5.33	1.45	1.52
1	A	364	MET	CB-CG	5.30	1.68	1.52
1	A	55	ASP	CA-C	-5.29	1.45	1.52
1	A	144	ARG	NE-CZ	5.29	1.38	1.33
1	A	105	ARG	NE-CZ	5.28	1.38	1.33
1	A	126	THR	C-O	-5.27	1.17	1.24
1	A	26	PRO	C-O	5.26	1.30	1.24
1	A	181	LEU	CA-C	5.26	1.59	1.52
1	A	436	ALA	CA-C	5.26	1.59	1.52
1	A	45	ASP	N-CA	5.24	1.52	1.45
1	A	409	SER	CA-C	5.20	1.58	1.52
1	A	269	LYS	CE-NZ	-5.18	1.33	1.49
1	A	209	PRO	CA-CB	-5.17	1.46	1.53
1	A	319	ASP	C-O	-5.17	1.18	1.24
1	A	372	THR	N-CA	5.15	1.52	1.46
1	A	425	VAL	CA-CB	-5.15	1.47	1.54
1	A	346	ALA	C-O	-5.12	1.18	1.24
1	A	92	TYR	CD2-CE2	5.11	1.53	1.38
1	A	15	VAL	C-O	-5.11	1.18	1.24
1	A	135	ALA	N-CA	-5.10	1.40	1.46
1	A	196	ALA	C-O	-5.08	1.17	1.24
1	A	286	VAL	C-O	-5.06	1.18	1.24
1	A	242	GLU	C-O	5.04	1.30	1.24
1	A	241	ASP	N-CA	5.03	1.53	1.46
1	A	130	LEU	CA-C	5.02	1.59	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	PHE	CB-CA-C	-9.22	93.69	109.83
1	A	145	PHE	N-CA-C	8.44	123.00	110.52
1	A	92	TYR	CA-C-N	7.62	136.09	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	TYR	C-N-CA	7.62	136.09	121.54
1	A	93	ALA	CA-C-N	6.99	129.65	120.28
1	A	93	ALA	C-N-CA	6.99	129.65	120.28
1	A	389	MET	CG-SD-CE	-6.66	86.25	100.90
1	A	93	ALA	N-CA-C	6.58	124.81	110.80
1	A	95	SER	N-CA-C	-6.35	97.27	110.80
1	A	222	SER	N-CA-C	-6.32	104.49	111.82
1	A	244	ILE	N-CA-C	6.09	118.04	111.58
1	A	20	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	A	24	VAL	CB-CA-C	5.93	117.02	110.62
1	A	347	ARG	CA-CB-CG	5.87	125.83	114.10
1	A	94	ALA	CA-C-O	5.55	126.44	120.55
1	A	188	ILE	CB-CA-C	-5.54	104.78	112.04
1	A	20	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	A	93	ALA	O-C-N	5.52	129.93	122.59
1	A	146	GLU	N-CA-C	5.44	118.12	109.96
1	A	25	MET	CG-SD-CE	-5.33	89.16	100.90
1	A	352	TRP	N-CA-C	-5.31	101.11	109.50
1	A	287	MET	N-CA-C	-5.26	105.72	111.82
1	A	248	ARG	CG-CD-NE	5.15	123.33	112.00
1	A	140	ARG	N-CA-CB	-5.12	103.56	110.67
1	A	347	ARG	N-CA-CB	-5.12	102.39	110.06
1	A	357	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	A	99	GLU	N-CA-C	-5.08	105.83	111.36
1	A	104	GLU	N-CA-C	5.05	116.79	111.28
1	A	60	LEU	N-CA-C	-5.04	101.09	109.46
1	A	177	THR	N-CA-C	5.03	118.52	112.38
1	A	121	SER	CA-C-N	5.03	125.53	120.00
1	A	121	SER	C-N-CA	5.03	125.53	120.00

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	3055	0	3013	53	0
2	A	130	0	0	4	0
All	All	3185	0	3013	53	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 9.

All (53) 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:389:MET:SD	1:A:389:MET:CE	2.02	1.47
1:A:389:MET:CE	1:A:389:MET:CG	2.59	0.81
1:A:145:PHE:CD2	1:A:145:PHE:N	2.48	0.76
1:A:94:ALA:O	1:A:95:SER:OG	2.07	0.73
1:A:379:ARG:HD2	1:A:381:GLU:OE1	1.90	0.71
1:A:275:LEU:HB3	1:A:276:PRO:HD2	1.74	0.69
1:A:112:SER:HB2	1:A:261:GLN:OE1	1.92	0.69
1:A:96:HIS:HD2	1:A:98:LEU:H	1.42	0.67
1:A:335:GLN:NE2	1:A:338:ARG:HH21	1.96	0.64
1:A:145:PHE:N	1:A:145:PHE:HD2	1.94	0.60
1:A:353:LEU:CD1	1:A:355:TYR:HB3	2.32	0.59
1:A:112:SER:HB3	1:A:255:GLN:OE1	2.03	0.58
1:A:248:ARG:HD3	1:A:359:SER:OG	2.04	0.57
1:A:356:GLY:HA2	2:A:553:HOH:O	2.04	0.57
1:A:291:SER:C	1:A:292:ARG:HD3	2.30	0.56
1:A:389:MET:CE	1:A:389:MET:HG3	2.36	0.56
1:A:292:ARG:HH11	1:A:292:ARG:HG3	1.70	0.56
1:A:280:LEU:HD13	1:A:287:MET:HE1	1.87	0.55
1:A:99:GLU:OE1	1:A:305:THR:HG22	2.07	0.55
1:A:25:MET:O	1:A:26:PRO:C	2.49	0.54
1:A:331:ASN:ND2	2:A:494:HOH:O	2.41	0.54
1:A:417:GLU:H	1:A:420:HIS:HD2	1.54	0.53
1:A:62:PHE:HB3	1:A:410:VAL:HB	1.90	0.52
1:A:293:GLY:O	1:A:294:SER:OG	2.23	0.52
1:A:195:PHE:O	1:A:199:GLY:HA3	2.09	0.51
1:A:146:GLU:OE2	1:A:147:GLY:HA3	2.12	0.49
1:A:96:HIS:CD2	1:A:98:LEU:H	2.26	0.47
1:A:218:PRO:O	1:A:378:THR:HG22	2.16	0.46
1:A:209:PRO:HB2	1:A:254:MET:HG2	1.99	0.45
1:A:60:LEU:HD13	1:A:62:PHE:CE2	2.51	0.45
1:A:260:VAL:HG12	1:A:261:GLN:N	2.32	0.45
1:A:275:LEU:HB3	1:A:276:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:THR:CG2	2:A:521:HOH:O	2.65	0.45
1:A:141:MET:HE1	1:A:179:ASN:ND2	2.33	0.44
1:A:94:ALA:C	1:A:95:SER:HG	2.16	0.44
1:A:287:MET:HE3	1:A:290:LEU:HD12	1.98	0.43
1:A:145:PHE:HE2	1:A:205:PHE:CZ	2.36	0.43
1:A:389:MET:HG3	1:A:440:LEU:O	2.19	0.43
1:A:293:GLY:O	1:A:294:SER:CB	2.66	0.43
1:A:353:LEU:HD11	1:A:355:TYR:HB3	2.00	0.42
1:A:91:GLN:O	1:A:307:ASN:ND2	2.53	0.42
1:A:275:LEU:HD12	1:A:310:THR:HA	2.01	0.42
1:A:63:PHE:CD1	1:A:405:GLY:HA3	2.55	0.42
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.83	0.41
1:A:93:ALA:HB1	1:A:96:HIS:HB2	2.02	0.41
1:A:117:ARG:NH2	1:A:291:SER:OG	2.47	0.41
1:A:330:ILE:HD13	1:A:330:ILE:HG21	1.90	0.41
1:A:60:LEU:HD12	1:A:423:HIS:HD2	1.85	0.41
1:A:140:ARG:HD2	2:A:580:HOH:O	2.21	0.40
1:A:335:GLN:HE21	1:A:338:ARG:HH21	1.69	0.40
1:A:283:ARG:O	1:A:287:MET:HB2	2.21	0.40
1:A:417:GLU:H	1:A:420:HIS:CD2	2.35	0.40
1:A:141:MET:CE	1:A:179:ASN:ND2	2.84	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	394/453 (87%)	370 (94%)	19 (5%)	5 (1%)	9 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ALA
1	A	444	GLN
1	A	27	ASP
1	A	26	PRO
1	A	38	PRO

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	311/353 (88%)	279 (90%)	32 (10%)	7 8

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	27	ASP
1	A	36	PHE
1	A	41	LEU
1	A	60	LEU
1	A	71	LEU
1	A	77	ARG
1	A	91	GLN
1	A	97	PRO
1	A	99	GLU
1	A	127	LEU
1	A	130	LEU
1	A	142	ILE
1	A	145	PHE
1	A	176	THR
1	A	183	ILE
1	A	248	ARG
1	A	280	LEU
1	A	284	GLU
1	A	287	MET
1	A	289	VAL
1	A	292	ARG

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Mol	Chain	Res	Type
1	A	305	THR
1	A	309	ILE
1	A	338	ARG
1	A	344	LEU
1	A	353	LEU
1	A	357	ARG
1	A	372	THR
1	A	384	ARG
1	A	410	VAL
1	A	439	ASN

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	5	ASN
1	A	50	HIS
1	A	79	ASN
1	A	91	GLN
1	A	96	HIS
1	A	179	ASN
1	A	251	ASN
1	A	331	ASN
1	A	335	GLN
1	A	415	GLN
1	A	420	HIS
1	A	423	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

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	402/453 (88%)	0.25	33 (8%) 17 19	23, 36, 73, 98	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	ALA	12.2
1	A	446	THR	7.1
1	A	93	ALA	6.8
1	A	445	GLY	6.6
1	A	35	ALA	6.2
1	A	36	PHE	5.7
1	A	92	TYR	5.0
1	A	177	THR	4.8
1	A	304	PHE	4.4
1	A	291	SER	4.4
1	A	305	THR	4.1
1	A	444	GLN	4.1
1	A	294	SER	4.1
1	A	145	PHE	3.9
1	A	176	THR	3.7
1	A	146	GLU	3.7
1	A	147	GLY	3.6
1	A	28	GLY	3.4
1	A	293	GLY	3.3
1	A	178	ALA	3.2
1	A	443	TRP	2.8
1	A	306	GLY	2.8
1	A	292	ARG	2.7
1	A	38	PRO	2.6
1	A	442	SER	2.3
1	A	27	ASP	2.3
1	A	37	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	200	SER	2.2
1	A	196	ALA	2.2
1	A	64	GLY	2.1
1	A	138	GLY	2.1
1	A	26	PRO	2.1
1	A	384	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.