



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:47 AM UTC

PDB ID : 5IIP / pdb_00005iip
Title : Staphylococcus aureus OpuCA
Authors : Tosi, T.; Campeotto, I.; Freemont, P.S.; Grundling, A.
Deposited on : 2016-03-01
Resolution : 2.50 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

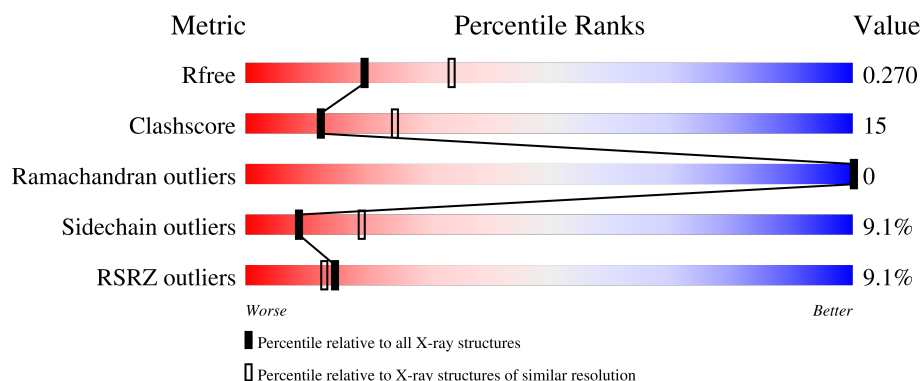
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	194	6% 43% 14% .. 40%
1	B	194	8% 35% 21% . 41%
1	C	194	4% 34% 24% . 40%
1	D	194	4% 42% 16% .. 40%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3732 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 Glycine betaine/carnitine/choline ABC transporter%2C ATP-binding protein%2C putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	97	0	0
			929	580	172	174	3			
1	B	115	Total	C	N	O	S	70	0	0
			917	570	168	176	3			
1	C	116	Total	C	N	O	S	78	0	0
			929	580	171	175	3			
1	D	117	Total	C	N	O	S	68	0	0
			942	590	174	175	3			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	GLY	-	expression tag	UNP A0A0D6GYR3
A	216	SER	-	expression tag	UNP A0A0D6GYR3
A	217	SER	-	expression tag	UNP A0A0D6GYR3
A	218	HIS	-	expression tag	UNP A0A0D6GYR3
A	219	HIS	-	expression tag	UNP A0A0D6GYR3
A	220	HIS	-	expression tag	UNP A0A0D6GYR3
A	221	HIS	-	expression tag	UNP A0A0D6GYR3
A	222	HIS	-	expression tag	UNP A0A0D6GYR3
A	223	HIS	-	expression tag	UNP A0A0D6GYR3
A	224	SER	-	expression tag	UNP A0A0D6GYR3
A	225	SER	-	expression tag	UNP A0A0D6GYR3
A	226	GLY	-	expression tag	UNP A0A0D6GYR3
A	227	LEU	-	expression tag	UNP A0A0D6GYR3
A	228	VAL	-	expression tag	UNP A0A0D6GYR3
A	229	PRO	-	expression tag	UNP A0A0D6GYR3
A	230	ARG	-	expression tag	UNP A0A0D6GYR3
A	231	GLY	-	expression tag	UNP A0A0D6GYR3
A	232	SER	-	expression tag	UNP A0A0D6GYR3
A	233	HIS	-	expression tag	UNP A0A0D6GYR3
A	234	MET	-	expression tag	UNP A0A0D6GYR3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	235	ALA	-	expression tag	UNP A0A0D6GYR3
A	236	SER	-	expression tag	UNP A0A0D6GYR3
B	215	GLY	-	expression tag	UNP A0A0D6GYR3
B	216	SER	-	expression tag	UNP A0A0D6GYR3
B	217	SER	-	expression tag	UNP A0A0D6GYR3
B	218	HIS	-	expression tag	UNP A0A0D6GYR3
B	219	HIS	-	expression tag	UNP A0A0D6GYR3
B	220	HIS	-	expression tag	UNP A0A0D6GYR3
B	221	HIS	-	expression tag	UNP A0A0D6GYR3
B	222	HIS	-	expression tag	UNP A0A0D6GYR3
B	223	HIS	-	expression tag	UNP A0A0D6GYR3
B	224	SER	-	expression tag	UNP A0A0D6GYR3
B	225	SER	-	expression tag	UNP A0A0D6GYR3
B	226	GLY	-	expression tag	UNP A0A0D6GYR3
B	227	LEU	-	expression tag	UNP A0A0D6GYR3
B	228	VAL	-	expression tag	UNP A0A0D6GYR3
B	229	PRO	-	expression tag	UNP A0A0D6GYR3
B	230	ARG	-	expression tag	UNP A0A0D6GYR3
B	231	GLY	-	expression tag	UNP A0A0D6GYR3
B	232	SER	-	expression tag	UNP A0A0D6GYR3
B	233	HIS	-	expression tag	UNP A0A0D6GYR3
B	234	MET	-	expression tag	UNP A0A0D6GYR3
B	235	ALA	-	expression tag	UNP A0A0D6GYR3
B	236	SER	-	expression tag	UNP A0A0D6GYR3
C	215	GLY	-	expression tag	UNP A0A0D6GYR3
C	216	SER	-	expression tag	UNP A0A0D6GYR3
C	217	SER	-	expression tag	UNP A0A0D6GYR3
C	218	HIS	-	expression tag	UNP A0A0D6GYR3
C	219	HIS	-	expression tag	UNP A0A0D6GYR3
C	220	HIS	-	expression tag	UNP A0A0D6GYR3
C	221	HIS	-	expression tag	UNP A0A0D6GYR3
C	222	HIS	-	expression tag	UNP A0A0D6GYR3
C	223	HIS	-	expression tag	UNP A0A0D6GYR3
C	224	SER	-	expression tag	UNP A0A0D6GYR3
C	225	SER	-	expression tag	UNP A0A0D6GYR3
C	226	GLY	-	expression tag	UNP A0A0D6GYR3
C	227	LEU	-	expression tag	UNP A0A0D6GYR3
C	228	VAL	-	expression tag	UNP A0A0D6GYR3
C	229	PRO	-	expression tag	UNP A0A0D6GYR3
C	230	ARG	-	expression tag	UNP A0A0D6GYR3
C	231	GLY	-	expression tag	UNP A0A0D6GYR3
C	232	SER	-	expression tag	UNP A0A0D6GYR3

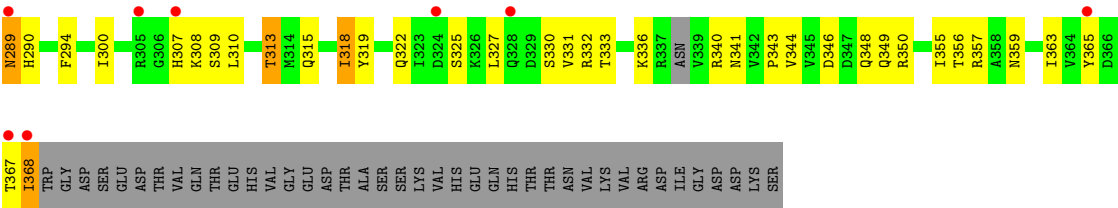
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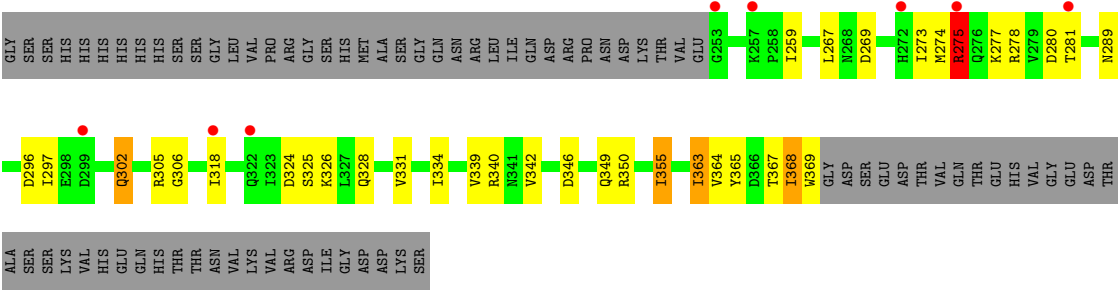
Chain	Residue	Modelled	Actual	Comment	Reference
C	233	HIS	-	expression tag	UNP A0A0D6GYR3
C	234	MET	-	expression tag	UNP A0A0D6GYR3
C	235	ALA	-	expression tag	UNP A0A0D6GYR3
C	236	SER	-	expression tag	UNP A0A0D6GYR3
D	215	GLY	-	expression tag	UNP A0A0D6GYR3
D	216	SER	-	expression tag	UNP A0A0D6GYR3
D	217	SER	-	expression tag	UNP A0A0D6GYR3
D	218	HIS	-	expression tag	UNP A0A0D6GYR3
D	219	HIS	-	expression tag	UNP A0A0D6GYR3
D	220	HIS	-	expression tag	UNP A0A0D6GYR3
D	221	HIS	-	expression tag	UNP A0A0D6GYR3
D	222	HIS	-	expression tag	UNP A0A0D6GYR3
D	223	HIS	-	expression tag	UNP A0A0D6GYR3
D	224	SER	-	expression tag	UNP A0A0D6GYR3
D	225	SER	-	expression tag	UNP A0A0D6GYR3
D	226	GLY	-	expression tag	UNP A0A0D6GYR3
D	227	LEU	-	expression tag	UNP A0A0D6GYR3
D	228	VAL	-	expression tag	UNP A0A0D6GYR3
D	229	PRO	-	expression tag	UNP A0A0D6GYR3
D	230	ARG	-	expression tag	UNP A0A0D6GYR3
D	231	GLY	-	expression tag	UNP A0A0D6GYR3
D	232	SER	-	expression tag	UNP A0A0D6GYR3
D	233	HIS	-	expression tag	UNP A0A0D6GYR3
D	234	MET	-	expression tag	UNP A0A0D6GYR3
D	235	ALA	-	expression tag	UNP A0A0D6GYR3
D	236	SER	-	expression tag	UNP A0A0D6GYR3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	3	Total O 3 3	0	0
2	C	3	Total O 3 3	0	0
2	D	7	Total O 7 7	0	0



● Molecule 1: Glycine betaine/carnitine/choline ABC transporter%2C ATP-binding protein%2C putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.15Å 88.26Å 61.79Å 90.00° 114.79° 90.00°	Depositor
Resolution (Å)	47.34 – 2.50 47.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.34-2.50) 99.9 (47.34-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.280 0.249 , 0.270	Depositor DCC
R_{free} test set	882 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3732	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.83	5/938 (0.5%)	1.20	5/1270 (0.4%)
1	B	1.77	5/923 (0.5%)	1.14	3/1246 (0.2%)
1	C	1.79	4/937 (0.4%)	1.16	5/1267 (0.4%)
1	D	1.79	2/953 (0.2%)	1.22	9/1292 (0.7%)
All	All	1.79	16/3751 (0.4%)	1.18	22/5075 (0.4%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	GLY	C-O	-6.64	1.17	1.23
1	D	355	ILE	C-O	-5.93	1.17	1.24
1	B	261	ILE	C-O	-5.79	1.18	1.24
1	C	344	VAL	C-O	-5.75	1.17	1.24
1	C	355	ILE	C-O	-5.58	1.18	1.24
1	B	353	GLY	C-O	-5.57	1.18	1.23
1	B	355	ILE	C-O	-5.45	1.18	1.24
1	C	278	ARG	CA-C	-5.42	1.46	1.53
1	A	282	ILE	C-O	-5.42	1.18	1.24
1	C	315	GLN	CA-C	-5.32	1.46	1.52
1	D	334	ILE	C-O	-5.24	1.18	1.24
1	A	260	THR	CA-C	-5.19	1.46	1.52
1	A	318	ILE	C-O	-5.18	1.18	1.23
1	B	291	LEU	C-O	-5.17	1.17	1.24
1	A	284	VAL	C-O	-5.14	1.18	1.24
1	B	354	LEU	C-O	-5.04	1.18	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	340	ARG	N-CA-C	8.93	121.09	111.36
1	A	281	THR	N-CA-C	7.91	121.48	109.23
1	B	254	VAL	N-CA-C	7.32	120.24	111.09
1	D	368	ILE	N-CA-C	-7.09	102.32	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	363	ILE	CB-CA-C	-7.04	102.96	111.97
1	B	273	ILE	N-CA-C	6.93	117.72	110.72
1	B	263	ALA	N-CA-C	6.87	118.77	111.28
1	D	368	ILE	CB-CA-C	-6.57	104.36	111.59
1	C	277	LYS	N-CA-C	-6.50	98.65	109.24
1	A	320	THR	N-CA-C	5.89	118.65	109.52
1	C	289	ASN	N-CA-C	5.85	119.71	112.58
1	A	330	SER	N-CA-C	-5.78	105.54	112.59
1	D	331	VAL	N-CA-C	5.66	116.40	110.62
1	A	341	ASN	N-CA-C	5.61	118.25	108.76
1	A	335	LEU	N-CA-C	5.50	117.35	111.36
1	C	341	ASN	N-CA-C	5.49	117.85	108.90
1	D	306	GLY	N-CA-C	-5.49	107.78	114.92
1	C	318	ILE	CB-CA-C	-5.27	102.53	110.55
1	D	297	ILE	N-CA-C	5.14	115.87	110.62
1	D	275	ARG	CB-CG-CD	5.12	123.08	111.30
1	D	280	ASP	N-CA-C	5.11	116.93	111.36
1	C	279	VAL	N-CA-C	5.03	116.95	108.81

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	929	0	958	20	16
1	B	917	0	934	36	8
1	C	929	0	957	32	23
1	D	942	0	966	19	1
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	7	0	0	0	0
All	All	3732	0	3815	104	24

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 15.

All (104) 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:281:THR:HG21	1:A:294:PHE:CE1	1.36	1.55
1:A:281:THR:CG2	1:A:294:PHE:HE1	1.27	1.48
1:C:254:VAL:HG13	1:C:363:ILE:CD1	1.48	1.42
1:A:281:THR:CG2	1:A:294:PHE:CE1	2.05	1.30
1:C:254:VAL:HG13	1:C:363:ILE:HD12	1.32	1.11
1:A:274:MET:HE1	1:A:297:ILE:HG12	1.13	1.10
1:C:254:VAL:CG1	1:C:363:ILE:CD1	2.32	1.07
1:C:254:VAL:CG1	1:C:363:ILE:HD12	1.89	1.01
1:D:365:TYR:O	1:D:368:ILE:O	1.81	0.98
1:C:274:MET:O	1:C:277:LYS:O	1.81	0.96
1:C:254:VAL:HG13	1:C:363:ILE:HD13	1.51	0.91
1:A:274:MET:CE	1:A:297:ILE:HG12	2.02	0.85
1:A:337:ARG:NH1	1:D:296:ASP:OD2	2.13	0.81
1:C:254:VAL:HG13	1:C:363:ILE:HD11	1.60	0.79
1:B:309:SER:O	1:B:313:THR:HG22	1.84	0.77
1:A:252:GLU:OE1	1:A:252:GLU:N	2.18	0.75
1:D:274:MET:CE	1:D:281:THR:HA	2.16	0.75
1:B:274:MET:HE2	1:B:300:ILE:CD1	2.16	0.74
1:A:281:THR:HG22	1:A:294:PHE:CE1	2.19	0.74
1:B:274:MET:HE2	1:B:300:ILE:HD11	1.70	0.73
1:D:274:MET:HE3	1:D:281:THR:HA	1.71	0.73
1:B:330:SER:O	1:B:334:ILE:HD13	1.89	0.72
1:C:269:ASP:O	1:C:273:ILE:HG13	1.95	0.68
1:C:356:THR:OG1	1:C:359:ASN:OD1	2.12	0.67
1:C:322:GLN:O	1:C:325:SER:OG	2.13	0.67
1:B:327:LEU:O	1:B:331:VAL:HG23	1.95	0.66
1:C:346:ASP:OD2	1:C:350:ARG:HB2	1.97	0.65
1:C:254:VAL:CG1	1:C:363:ILE:HD13	2.18	0.65
1:B:250:THR:HA	1:B:327:LEU:HB2	1.77	0.64
1:D:363:ILE:O	1:D:367:THR:OG1	2.12	0.63
1:B:334:ILE:HG13	1:B:342:VAL:HG21	1.80	0.63
1:A:281:THR:HG21	1:A:294:PHE:HE1	0.48	0.63
1:B:322:GLN:O	1:B:325:SER:OG	2.17	0.62
1:D:302:GLN:O	1:D:305:ARG:O	2.18	0.62
1:B:333:THR:O	1:B:337:ARG:HG2	1.99	0.62
1:B:250:THR:HG23	1:B:251:VAL:H	1.64	0.62
1:B:365:TYR:O	1:B:368:ILE:HG13	2.00	0.61
1:C:365:TYR:C	1:C:367:THR:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ILE:HG13	1:B:342:VAL:CG2	2.32	0.60
1:C:346:ASP:CG	1:C:350:ARG:HB2	2.27	0.60
1:C:327:LEU:O	1:C:331:VAL:HG23	2.03	0.59
1:C:283:PHE:CE1	1:C:343:PRO:HG3	2.39	0.58
1:B:267:LEU:H	1:B:267:LEU:HD12	1.69	0.58
1:C:270:ALA:O	1:C:274:MET:HG3	2.04	0.57
1:D:368:ILE:HG22	1:D:369:TRP:N	2.18	0.57
1:B:334:ILE:CD1	1:B:342:VAL:HG21	2.35	0.57
1:C:332:ARG:O	1:C:336:LYS:HG3	2.06	0.56
1:C:348:GLN:O	1:C:349:GLN:HB2	2.04	0.56
1:A:281:THR:HG21	1:A:294:PHE:CZ	2.24	0.56
1:A:337:ARG:HH12	1:D:296:ASP:CG	2.13	0.56
1:C:254:VAL:HG12	1:C:254:VAL:O	2.06	0.55
1:B:274:MET:HE2	1:B:300:ILE:HD12	1.89	0.54
1:B:274:MET:CE	1:B:300:ILE:HD12	2.36	0.54
1:D:274:MET:O	1:D:278:ARG:N	2.40	0.54
1:D:339:VAL:O	1:D:339:VAL:HG23	2.07	0.54
1:C:309:SER:O	1:C:313:THR:HG22	2.08	0.54
1:C:340:ARG:HD2	1:C:357:ARG:HB3	1.90	0.53
1:B:296:ASP:O	1:B:300:ILE:HG13	2.08	0.53
1:D:346:ASP:OD2	1:D:350:ARG:HB2	2.08	0.53
1:D:274:MET:O	1:D:278:ARG:HA	2.08	0.53
1:B:302:GLN:O	1:B:306:GLY:HA3	2.09	0.53
1:B:250:THR:CG2	1:B:251:VAL:N	2.72	0.53
1:B:330:SER:O	1:B:334:ILE:CD1	2.57	0.52
1:C:330:SER:O	1:C:333:THR:HG22	2.11	0.51
1:B:334:ILE:N	1:B:334:ILE:HD12	2.26	0.51
1:D:259:ILE:HD12	1:D:277:LYS:HG2	1.93	0.51
1:B:334:ILE:CG1	1:B:342:VAL:HG21	2.41	0.50
1:B:261:ILE:HD13	1:B:310:LEU:HD11	1.92	0.50
1:B:267:LEU:HD11	1:B:309:SER:HA	1.93	0.50
1:B:250:THR:HG23	1:B:251:VAL:N	2.26	0.50
1:D:342:VAL:HB	1:D:355:ILE:CG1	2.42	0.49
1:A:366:ASP:OD1	1:C:307:HIS:NE2	2.35	0.49
1:B:274:MET:O	1:B:278:ARG:C	2.55	0.49
1:A:274:MET:O	1:A:278:ARG:N	2.46	0.49
1:B:326:LYS:HD2	1:B:326:LYS:H	1.78	0.48
1:C:318:ILE:HG22	1:C:319:TYR:N	2.28	0.48
1:B:274:MET:CE	1:B:300:ILE:CD1	2.89	0.47
1:C:286:ASP:OD2	1:C:290:HIS:HB2	2.15	0.47
1:B:332:ARG:HH11	1:B:332:ARG:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:HG22	1:A:358:ALA:H	1.80	0.47
1:A:281:THR:HG23	1:A:295:LEU:O	2.15	0.46
1:A:267:LEU:O	1:A:271:VAL:HG23	2.16	0.46
1:D:342:VAL:HB	1:D:355:ILE:HG12	1.97	0.46
1:C:346:ASP:OD2	1:C:350:ARG:NE	2.49	0.46
1:B:326:LYS:HD2	1:B:326:LYS:N	2.31	0.45
1:A:281:THR:CG2	1:A:294:PHE:CD1	2.86	0.45
1:C:288:ASN:O	1:C:289:ASN:HB2	2.15	0.45
1:C:319:TYR:OH	1:C:333:THR:HG21	2.17	0.45
1:C:327:LEU:HG	1:C:331:VAL:CG2	2.47	0.45
1:A:254:VAL:O	1:A:254:VAL:HG22	2.18	0.44
1:B:332:ARG:HG2	1:B:332:ARG:NH1	2.33	0.44
1:D:259:ILE:CD1	1:D:277:LYS:HG2	2.48	0.44
1:A:281:THR:HG22	1:A:294:PHE:CD1	2.50	0.44
1:B:255:MET:HE1	1:B:352:VAL:HG12	2.00	0.43
1:B:251:VAL:HG13	1:B:355:ILE:HD11	2.00	0.43
1:B:334:ILE:HD11	1:B:342:VAL:HG21	2.00	0.43
1:D:346:ASP:CG	1:D:350:ARG:HB2	2.44	0.43
1:C:254:VAL:HG11	1:C:363:ILE:HD12	1.89	0.42
1:D:269:ASP:O	1:D:273:ILE:HG13	2.19	0.41
1:A:333:THR:O	1:A:337:ARG:HG3	2.21	0.41
1:B:293:GLY:HA2	1:B:318:ILE:HD11	2.02	0.41
1:C:267:LEU:O	1:C:271:VAL:HG23	2.20	0.41
1:D:267:LEU:HD23	1:D:267:LEU:HA	1.91	0.41
1:B:359:ASN:O	1:B:363:ILE:HG13	2.20	0.40

All (24) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TYR:CE1	1:C:332:ARG:NH2[1_655]	0.49	1.71
1:A:365:TYR:CG	1:C:332:ARG:NH1[1_655]	0.69	1.51
1:B:275:ARG:NH2	1:C:368:ILE:O[2_456]	0.71	1.49
1:B:275:ARG:NH2	1:C:368:ILE:C[2_456]	0.72	1.48
1:B:275:ARG:CZ	1:C:368:ILE:O[2_456]	0.85	1.35
1:A:365:TYR:CD1	1:C:332:ARG:NH2[1_655]	1.03	1.17
1:A:365:TYR:CD2	1:C:332:ARG:NH1[1_655]	1.10	1.10
1:A:365:TYR:CD1	1:C:332:ARG:CZ[1_655]	1.33	0.87
1:A:365:TYR:CZ	1:C:332:ARG:NH2[1_655]	1.41	0.79
1:A:365:TYR:CG	1:C:332:ARG:CZ[1_655]	1.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TYR:CE1	1:C:332:ARG:CZ[1_655]	1.55	0.65
1:A:365:TYR:CD2	1:C:332:ARG:CZ[1_655]	1.63	0.57
1:A:365:TYR:CB	1:C:332:ARG:NH1[1_655]	1.64	0.56
1:A:365:TYR:CZ	1:C:332:ARG:CZ[1_655]	1.78	0.42
1:B:275:ARG:NH2	1:C:368:ILE:CA[2_456]	1.79	0.41
1:A:365:TYR:CE2	1:C:332:ARG:CZ[1_655]	1.82	0.38
1:A:365:TYR:CD1	1:C:332:ARG:NH1[1_655]	1.83	0.37
1:B:275:ARG:NE	1:C:368:ILE:O[2_456]	1.84	0.36
1:B:275:ARG:NH1	1:C:368:ILE:O[2_456]	1.88	0.32
1:A:365:TYR:CG	1:C:332:ARG:NH2[1_655]	1.92	0.28
1:A:347:ASP:OD2	1:C:288:ASN:ND2[1_554]	1.93	0.27
1:B:275:ARG:CZ	1:C:368:ILE:C[2_456]	1.97	0.23
1:A:365:TYR:CE2	1:C:332:ARG:NH2[1_655]	2.14	0.06
1:B:289:ASN:ND2	1:D:275:ARG:NH2[2_656]	2.16	0.04

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	114/194 (59%)	110 (96%)	4 (4%)	0	100	100
1	B	107/194 (55%)	104 (97%)	3 (3%)	0	100	100
1	C	112/194 (58%)	109 (97%)	3 (3%)	0	100	100
1	D	115/194 (59%)	115 (100%)	0	0	100	100
All	All	448/776 (58%)	438 (98%)	10 (2%)	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	107/176 (61%)	97 (91%)	10 (9%)	8	18
1	B	106/176 (60%)	95 (90%)	11 (10%)	7	14
1	C	107/176 (61%)	99 (92%)	8 (8%)	12	26
1	D	108/176 (61%)	98 (91%)	10 (9%)	8	18
All	All	428/704 (61%)	389 (91%)	39 (9%)	9	19

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	GLU
1	A	257	LYS
1	A	278	ARG
1	A	281	THR
1	A	298	GLU
1	A	302	GLN
1	A	316	GLN
1	A	324	ASP
1	A	333	THR
1	A	363	ILE
1	B	250	THR
1	B	252	GLU
1	B	257	LYS
1	B	264	GLU
1	B	274	MET
1	B	278	ARG
1	B	281	THR
1	B	284	VAL
1	B	307	HIS
1	B	326	LYS
1	B	330	SER
1	C	252	GLU
1	C	282	ILE
1	C	294	PHE
1	C	300	ILE
1	C	308	LYS
1	C	310	LEU
1	C	313	THR
1	C	368	ILE
1	D	275	ARG

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Mol	Chain	Res	Type
1	D	289	ASN
1	D	302	GLN
1	D	318	ILE
1	D	324	ASP
1	D	325	SER
1	D	326	LYS
1	D	328	GLN
1	D	349	GLN
1	D	364	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
1	A	290	HIS
1	B	341	ASN
1	B	359	ASN
1	C	322	GLN
1	D	272	HIS
1	D	301	ASN

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

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	115/194 (59%)	0.86	11 (9%) 13 11	15, 42, 65, 71	23 (20%)
1	B	115/194 (59%)	1.06	15 (13%) 7 6	18, 44, 65, 70	17 (14%)
1	C	116/194 (59%)	0.95	8 (6%) 23 20	18, 49, 63, 67	20 (17%)
1	D	117/194 (60%)	0.99	8 (6%) 23 20	22, 47, 63, 80	16 (13%)
All	All	463/776 (59%)	0.96	42 (9%) 15 13	15, 45, 64, 80	76 (16%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	ASP	4.7
1	C	368	ILE	4.6
1	D	253	GLY	4.1
1	C	289	ASN	3.9
1	B	301	ASN	3.8
1	A	302	GLN	3.5
1	C	324	ASP	3.4
1	A	327	LEU	3.3
1	A	339	VAL	3.2
1	B	277	LYS	3.2
1	B	303	GLY	3.2
1	A	330	SER	3.2
1	B	280	ASP	3.1
1	A	342	VAL	3.1
1	B	368	ILE	3.1
1	C	305	ARG	3.0
1	A	296	ASP	3.0
1	B	281	THR	2.9
1	C	365	TYR	2.8
1	B	264	GLU	2.7
1	D	272	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	281	THR	2.6
1	B	341	ASN	2.6
1	A	365	TYR	2.5
1	A	338	ASN	2.5
1	A	341	ASN	2.5
1	B	250	THR	2.5
1	B	328	GLN	2.5
1	B	284	VAL	2.4
1	C	328	GLN	2.4
1	D	275	ARG	2.3
1	D	322	GLN	2.3
1	D	318	ILE	2.3
1	B	306	GLY	2.3
1	B	298	GLU	2.3
1	D	299	ASP	2.2
1	A	364	VAL	2.2
1	C	367	THR	2.2
1	C	307	HIS	2.2
1	B	347	ASP	2.1
1	B	278	ARG	2.1
1	D	257	LYS	2.1

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.