



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:19 PM UTC

PDB ID : 2D1W / pdb_00002d1w
Title : Substrate Schiff-Base intermediate with tyramine in copper amine oxidase from *Arthrobacter globiformis*
Authors : Murakawa, T.; Okajima, T.; Kuroda, S.; Nakamoto, T.; Taki, M.; Yamamoto, Y.; Hayashi, H.; Tanizawa, K.
Deposited on : 2005-09-01
Resolution : 1.74 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

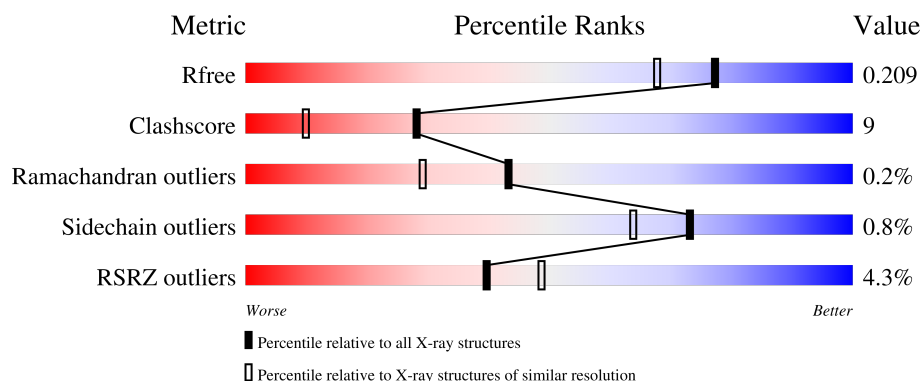
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	638	5% 77% 19% ..
1	B	638	4% 83% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10930 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	1	0
			4897	3098	858	932	9			
1	B	620	Total	C	N	O	S	0	1	0
			4897	3098	858	932	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	ALA	ASP	engineered mutation	UNP P46881
A	382	TTS	TYR	modified residue	UNP P46881
B	298	ALA	ASP	engineered mutation	UNP P46881
B	382	TTS	TYR	modified residue	UNP P46881

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	547	Total	O	0	0
			547	547		
3	B	587	Total	O	0	0
			587	587		

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.57Å 63.35Å 183.65Å 90.00° 112.29° 90.00°	Depositor
Resolution (Å)	26.44 – 1.74 26.44 – 1.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.44-1.74) 99.8 (26.44-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.74Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.217 0.184 , 0.209	Depositor DCC
R_{free} test set	8601 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10930	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8718e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TTS, CU

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	0.34	0/4972	0.91	14/6770 (0.2%)
1	B	0.34	0/4972	0.91	17/6770 (0.3%)
All	All	0.34	0/9944	0.91	31/13540 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	602	MET	N-CA-C	7.50	119.23	109.93
1	A	602	MET	N-CA-C	7.42	119.42	110.07
1	B	310	SER	N-CA-C	-6.67	99.04	109.25
1	A	294	GLN	N-CA-C	6.59	118.64	109.15
1	B	304	VAL	N-CA-C	6.09	116.83	110.62
1	B	224	GLN	CA-C-N	5.80	125.93	119.32
1	B	224	GLN	C-N-CA	5.80	125.93	119.32
1	A	582	ILE	N-CA-C	5.79	117.18	108.96
1	A	592	HIS	N-CA-C	5.79	117.95	108.52
1	B	300	GLY	N-CA-C	5.64	119.99	112.77
1	B	277	ILE	N-CA-C	-5.59	98.39	106.88
1	B	294	GLN	N-CA-C	5.58	117.19	109.15
1	A	374	SER	N-CA-C	5.48	117.12	108.96
1	A	304	VAL	N-CA-C	5.43	117.84	111.05
1	A	199	ALA	N-CA-C	5.36	118.28	111.69
1	B	455	VAL	N-CA-C	-5.36	102.67	109.80
1	A	408	THR	N-CA-C	5.36	118.02	110.14
1	B	295	ASN	CA-C-N	-5.31	115.68	123.00
1	B	295	ASN	C-N-CA	-5.31	115.68	123.00
1	B	582	ILE	N-CA-C	5.31	117.27	108.99
1	A	321	ILE	N-CA-C	5.26	116.56	108.71
1	B	592	HIS	N-CA-C	5.26	117.10	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	593	PHE	N-CA-C	-5.21	97.40	108.66
1	B	374	SER	N-CA-C	5.17	116.67	108.96
1	B	605	ASP	N-CA-C	-5.09	101.57	109.72
1	A	295	ASN	CA-C-N	-5.08	115.83	122.99
1	A	295	ASN	C-N-CA	-5.08	115.83	122.99
1	A	277	ILE	N-CA-C	-5.07	99.18	106.88
1	A	605	ASP	N-CA-C	-5.03	101.55	109.50
1	A	310	SER	N-CA-C	-5.03	100.96	108.96
1	B	410	ALA	N-CA-C	-5.03	103.07	110.52

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	4897	0	4711	98	0
1	B	4897	0	4709	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	547	0	0	6	0
3	B	587	0	0	4	0
All	All	10930	0	9420	170	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 (170) 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:B:168:TRP:HH2	1:B:382[A]:TTS:H5'	1.08	1.13
1:B:168:TRP:CH2	1:B:382[A]:TTS:H5'	2.00	0.95
1:A:238:ILE:HG13	1:A:344:MET:HE1	1.60	0.83
1:B:382[A]:TTS:O1	3:B:1411:HOH:O	1.97	0.81
1:B:341:GLY:C	1:B:342:ILE:HD12	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ASP:CG	1:B:214:ARG:HD2	2.13	0.73
1:B:422:LEU:HD11	1:B:428:ALA:HB2	1.71	0.72
1:A:104:GLU:O	1:A:107:VAL:HG22	1.90	0.71
1:B:328:ILE:HD13	1:B:336:ARG:O	1.91	0.70
1:B:326:PRO:HD3	1:B:342:ILE:HD13	1.74	0.69
1:A:505:ARG:HD3	1:A:618:ASP:HB3	1.76	0.68
1:A:22:GLU:O	1:A:26:ILE:HG12	1.94	0.68
1:A:206:ASP:CG	1:A:208:GLU:HG2	2.18	0.68
1:B:220:ILE:HG22	1:B:222:ILE:HD11	1.74	0.68
1:A:328:ILE:HD13	1:A:336:ARG:O	1.94	0.67
1:A:66:ASP:OD1	1:A:68:SER:HB3	1.95	0.67
1:A:168:TRP:HH2	1:A:382[A]:TTS:H5'	1.60	0.66
1:A:247:VAL:HG21	1:A:344:MET:HE3	1.78	0.65
1:A:180:ASP:OD1	1:A:182:VAL:HG22	1.97	0.65
1:A:33:LEU:HD11	1:A:39:ILE:HD11	1.79	0.64
1:A:170:HIS:HD2	1:A:198:PRO:O	1.81	0.64
1:A:187:THR:O	1:A:188:ARG:HG3	1.98	0.64
1:B:257:LEU:HB3	1:B:260:ILE:HD11	1.80	0.64
1:A:347:GLU:OE1	1:A:370:ARG:HD3	1.97	0.63
1:A:247:VAL:HG21	1:A:344:MET:CE	2.30	0.62
1:A:146:GLU:O	1:A:150:ARG:HD3	1.99	0.62
3:A:1174:HOH:O	1:B:621:PRO:HD2	1.99	0.62
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.35	0.62
1:A:206:ASP:OD1	1:A:208:GLU:HG2	2.00	0.62
1:A:137:LEU:HD12	1:A:293:TRP:HH2	1.64	0.61
1:B:146:GLU:O	1:B:150:ARG:HD3	2.00	0.61
1:B:530:ILE:HD13	1:B:530:ILE:O	2.00	0.61
1:A:238:ILE:CG1	1:A:344:MET:HE1	2.30	0.61
1:A:328:ILE:HD13	1:A:328:ILE:H	1.65	0.61
1:A:162:PHE:HB2	1:A:163:PRO:HD2	1.84	0.60
1:B:220:ILE:HG22	1:B:222:ILE:CD1	2.31	0.60
1:A:472:ARG:HD3	3:A:1490:HOH:O	2.01	0.59
1:B:290:ILE:HD12	1:B:290:ILE:N	2.17	0.59
1:A:261:ALA:HB1	1:A:268:LEU:HD22	1.85	0.58
1:A:260:ILE:HD12	1:A:260:ILE:N	2.17	0.58
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.38	0.58
1:A:443:ILE:H	1:A:448:ASN:HD21	1.53	0.57
1:B:328:ILE:HD13	1:B:328:ILE:H	1.69	0.57
1:A:526:PRO:HG3	3:B:1208:HOH:O	2.04	0.57
1:A:282:VAL:HB	1:A:296:TYR:CE2	2.40	0.57
1:A:483:ALA:HB1	1:A:543:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:HD12	1:B:342:ILE:N	2.20	0.57
1:A:72:PRO:HG2	1:A:90:LEU:HB2	1.85	0.56
1:B:106:GLU:O	1:B:110:GLN:HG3	2.05	0.56
1:A:432:GLN:HE22	1:A:523:LEU:H	1.53	0.56
1:B:39:ILE:HD12	1:B:39:ILE:N	2.22	0.55
1:A:222:ILE:HD12	1:A:222:ILE:N	2.22	0.55
1:A:144:TYR:CD2	1:A:188:ARG:NH1	2.76	0.54
1:B:222:ILE:HD12	1:B:222:ILE:N	2.22	0.54
1:A:277:ILE:HD12	1:A:277:ILE:N	2.22	0.54
1:B:530:ILE:HD13	1:B:530:ILE:C	2.33	0.54
1:A:324:LEU:HB2	1:A:342:ILE:HB	1.90	0.53
1:A:137:LEU:HD12	1:A:293:TRP:CH2	2.43	0.53
1:B:280:MET:CG	1:B:298:ALA:HB3	2.39	0.52
1:A:280:MET:HE1	1:A:384:TYR:CE2	2.45	0.52
1:A:321:ILE:N	1:A:321:ILE:HD12	2.25	0.51
1:A:220:ILE:HG22	1:A:222:ILE:HD11	1.92	0.51
1:B:245:LEU:HB2	1:B:260:ILE:HD13	1.92	0.51
1:B:379:ILE:O	1:B:382[A]:TTS:HD2	2.10	0.51
1:A:145:ALA:O	1:A:148:ARG:HD3	2.11	0.51
1:A:271:ILE:HG22	1:A:272:ILE:HG13	1.93	0.51
1:A:246:ASP:HB2	1:A:258:HIS:HB2	1.93	0.51
1:B:326:PRO:CD	1:B:342:ILE:HD13	2.40	0.51
1:B:72:PRO:HG2	1:B:90:LEU:HB2	1.94	0.50
1:A:39:ILE:HD12	1:A:39:ILE:N	2.26	0.50
1:B:324:LEU:HB2	1:B:342:ILE:HB	1.94	0.49
1:A:182:VAL:HG23	1:A:183:SER:N	2.27	0.49
1:B:241:GLU:O	1:B:242:LYS:HB2	2.12	0.49
1:A:194:VAL:HG13	3:A:1041:HOH:O	2.13	0.49
1:A:460:MET:HE1	1:B:528:SER:HA	1.95	0.49
1:A:624:ASP:OD2	1:B:214:ARG:HD2	2.12	0.49
1:A:626:PRO:HG2	1:A:628:ASN:ND2	2.28	0.49
1:B:280:MET:HG3	1:B:298:ALA:HB3	1.95	0.49
1:B:297:PHE:HB2	1:B:301:GLU:HG3	1.94	0.49
1:B:379:ILE:O	1:B:382[B]:TTS:HD2	2.13	0.49
1:A:20:ILE:HD12	1:A:327:VAL:HG12	1.95	0.49
1:B:351:ILE:HD12	1:B:351:ILE:N	2.27	0.49
1:A:369:ARG:CZ	1:B:220:ILE:HD13	2.43	0.48
1:A:261:ALA:CB	1:A:268:LEU:HD22	2.42	0.48
1:A:319:GLY:C	1:A:321:ILE:HD12	2.38	0.48
1:A:379:ILE:O	1:A:382[B]:TTS:HD2	2.12	0.48
1:A:370:ARG:O	1:A:370:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PHE:HB2	1:A:301:GLU:HG3	1.96	0.48
1:A:183:SER:OG	1:A:185:GLU:HG2	2.13	0.48
1:B:522:LEU:HD11	1:B:530:ILE:HD12	1.96	0.48
1:B:317:CYS:HB3	1:B:321:ILE:HG12	1.95	0.48
1:B:380:GLY:HA3	1:B:382[B]:TTS:C6'	2.44	0.48
1:A:42:LEU:C	1:A:42:LEU:HD23	2.39	0.48
1:A:550:GLU:HG2	1:A:570:TYR:CE1	2.49	0.48
1:A:373:ILE:HD12	1:A:373:ILE:N	2.28	0.47
1:B:483:ALA:HB1	1:B:543:VAL:HB	1.96	0.47
1:B:267:ARG:HG2	1:B:267:ARG:HH11	1.80	0.47
1:B:418:ASN:C	1:B:419:ILE:HD12	2.39	0.47
1:B:369:ARG:HG3	3:B:1414:HOH:O	2.15	0.47
1:A:367:ARG:HD3	1:B:315:CYS:O	2.15	0.47
1:B:245:LEU:CB	1:B:260:ILE:HD13	2.45	0.47
1:A:136:PRO:HD2	1:A:382[B]:TTS:C4'	2.46	0.46
1:B:582:ILE:C	1:B:582:ILE:HD12	2.40	0.46
1:A:163:PRO:HG2	3:A:1362:HOH:O	2.14	0.46
1:B:282:VAL:HB	1:B:296:TYR:CD2	2.51	0.46
1:A:369:ARG:NH2	1:B:220:ILE:HD13	2.31	0.46
1:A:484:VAL:HG12	1:A:539:LYS:HG3	1.97	0.46
1:A:270:PRO:C	1:A:271:ILE:HD12	2.40	0.46
1:B:219:PRO:C	1:B:220:ILE:HD12	2.40	0.46
1:A:105:PHE:HB3	1:A:136:PRO:HG2	1.97	0.46
3:A:1134:HOH:O	1:B:351:ILE:HD13	2.16	0.46
1:A:145:ALA:O	1:A:148:ARG:CD	2.64	0.45
1:B:42:LEU:C	1:B:42:LEU:HD23	2.40	0.45
1:A:241:GLU:O	1:A:242:LYS:HB2	2.16	0.45
1:A:271:ILE:HD12	1:A:271:ILE:N	2.31	0.45
1:B:13:ARG:NH2	1:B:58:ARG:HG3	2.32	0.44
1:A:66:ASP:CG	1:A:70:ALA:HB3	2.43	0.44
1:B:220:ILE:HD12	1:B:220:ILE:N	2.32	0.44
1:B:490:ARG:HG3	1:B:490:ARG:HH11	1.82	0.44
1:B:220:ILE:CG2	1:B:222:ILE:HD11	2.45	0.44
1:A:152:ILE:CG2	1:A:153:LEU:N	2.80	0.44
1:A:71:ARG:HD3	1:A:89:GLU:HG2	1.98	0.44
1:A:282:VAL:HB	1:A:296:TYR:CD2	2.53	0.44
1:B:188:ARG:HD3	3:B:1306:HOH:O	2.18	0.44
1:B:328:ILE:HD13	1:B:328:ILE:N	2.33	0.44
1:A:33:LEU:HD11	1:A:39:ILE:CD1	2.46	0.43
1:A:603:PRO:HG2	3:A:1174:HOH:O	2.17	0.43
1:B:282:VAL:HB	1:B:296:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LYS:O	1:A:611:LEU:HA	2.18	0.43
1:B:56:GLU:OE2	1:B:58:ARG:HG2	2.18	0.43
1:B:190:ILE:HD12	1:B:190:ILE:N	2.34	0.43
1:B:296:TYR:OH	1:B:384:TYR:HE2	2.02	0.43
1:B:22:GLU:O	1:B:26:ILE:HG12	2.19	0.42
1:B:298:ALA:HB1	1:B:379:ILE:CD1	2.49	0.42
1:A:296:TYR:CE1	1:A:298:ALA:HB2	2.54	0.42
1:A:214:ARG:HE	1:B:624:ASP:CG	2.27	0.42
1:A:260:ILE:HD12	1:A:260:ILE:H	1.83	0.42
1:A:137:LEU:HD11	1:A:156:LEU:HD12	2.02	0.42
1:A:116:GLU:O	1:A:120:LYS:HG3	2.20	0.42
1:B:20:ILE:HD12	1:B:327:VAL:HG12	2.02	0.42
1:B:479:ARG:O	1:B:482:GLU:HG2	2.19	0.42
1:A:238:ILE:CD1	1:A:344:MET:HE1	2.50	0.42
1:A:277:ILE:HD11	1:A:398:PHE:CE1	2.55	0.42
1:A:318:LEU:C	1:A:321:ILE:HD11	2.45	0.41
1:B:290:ILE:HD12	1:B:290:ILE:H	1.85	0.41
1:B:434:ILE:HD13	1:B:589:GLY:HA3	2.02	0.41
1:B:282:VAL:HA	1:B:432:GLN:O	2.20	0.41
1:B:290:ILE:N	1:B:290:ILE:CD1	2.82	0.41
1:B:468:ASN:HD22	1:B:468:ASN:H	1.68	0.41
1:A:154:ARG:HD2	1:A:293:TRP:CE3	2.55	0.41
1:A:72:PRO:HB2	1:A:98:LEU:HD11	2.02	0.41
1:A:260:ILE:N	1:A:260:ILE:CD1	2.83	0.41
1:A:460:MET:HE2	1:A:466:ARG:C	2.45	0.41
1:B:342:ILE:N	1:B:342:ILE:CD1	2.83	0.41
1:B:189:VAL:C	1:B:190:ILE:HD12	2.45	0.41
1:B:280:MET:HG3	1:B:280:MET:O	2.21	0.41
1:B:451:GLU:HG2	1:B:476:VAL:HG22	2.02	0.41
1:B:546:TYR:CD1	1:B:546:TYR:C	2.99	0.41
1:A:447:THR:HG21	1:A:501:GLU:OE2	2.20	0.41
1:A:486:GLU:OE1	1:A:539:LYS:NZ	2.51	0.41
1:B:101:LEU:HB2	1:B:104:GLU:HG3	2.01	0.41
1:A:280:MET:HG3	1:A:435:PHE:CD2	2.56	0.41
1:B:282:VAL:HG21	1:B:296:TYR:CE2	2.55	0.41
1:A:146:GLU:OE1	1:A:188:ARG:NH1	2.54	0.41
1:A:257:LEU:HB3	1:A:260:ILE:HD11	2.03	0.41
1:A:330:ASP:OD2	1:A:330:ASP:C	2.64	0.41
1:A:238:ILE:HG13	1:A:344:MET:CE	2.42	0.40
1:A:319:GLY:O	1:A:321:ILE:HD12	2.21	0.40
1:A:269:ARG:O	1:A:271:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ILE:HD12	1:B:321:ILE:N	2.37	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	617/638 (97%)	594 (96%)	22 (4%)	1 (0%)	43	29
1	B	617/638 (97%)	590 (96%)	26 (4%)	1 (0%)	43	29
All	All	1234/1276 (97%)	1184 (96%)	48 (4%)	2 (0%)	43	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	B	52	GLY

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	512/528 (97%)	508 (99%)	4 (1%)	73	64
1	B	512/528 (97%)	508 (99%)	4 (1%)	73	64
All	All	1024/1056 (97%)	1016 (99%)	8 (1%)	73	64

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	268	LEU
1	A	328	ILE
1	A	376	PHE
1	B	328	ILE
1	B	342	ILE
1	B	376	PHE
1	B	530	ILE

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	110	GLN
1	A	170	HIS
1	A	306	GLN
1	A	345	HIS
1	A	418	ASN
1	A	432	GLN
1	A	458	GLN
1	A	507	ASN
1	A	515	HIS
1	A	628	ASN
1	B	73	GLN
1	B	110	GLN
1	B	224	GLN
1	B	306	GLN
1	B	340	ASN
1	B	418	ASN
1	B	421	GLN
1	B	458	GLN
1	B	468	ASN
1	B	507	ASN
1	B	519	GLN
1	B	628	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TTS	B	382[A]	1	22,24,25	2.36	10 (45%)	22,32,34	1.65	3 (13%)
1	TTS	A	382[B]	1	22,24,25	2.42	10 (45%)	22,32,34	1.63	3 (13%)
1	TTS	B	382[B]	1	22,24,25	2.44	10 (45%)	22,32,34	1.64	3 (13%)
1	TTS	A	382[A]	1	22,24,25	2.36	10 (45%)	22,32,34	1.65	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TTS	B	382[A]	1	-	3/11/28/30	0/2/2/2
1	TTS	A	382[B]	1	-	2/11/28/30	0/2/2/2
1	TTS	B	382[B]	1	-	2/11/28/30	0/2/2/2
1	TTS	A	382[A]	1	-	3/11/28/30	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382[B]	TTS	CE1-CZ	4.85	1.44	1.36
1	A	382[B]	TTS	CE1-CZ	4.83	1.44	1.36
1	A	382[A]	TTS	CE1-CZ	4.78	1.44	1.36
1	B	382[A]	TTS	CE1-CZ	4.76	1.44	1.36
1	B	382[B]	TTS	C5'-C4'	4.34	1.47	1.39
1	A	382[B]	TTS	C5'-C4'	4.29	1.47	1.39
1	A	382[A]	TTS	C5'-C4'	4.03	1.46	1.39
1	B	382[A]	TTS	C5'-C4'	4.01	1.46	1.39
1	B	382[B]	TTS	CD2-CG	3.92	1.44	1.34
1	A	382[B]	TTS	CD2-CG	3.91	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382[A]	TTS	CD2-CG	3.88	1.44	1.34
1	B	382[A]	TTS	OD1-CD1	3.88	1.34	1.24
1	A	382[A]	TTS	CD2-CG	3.87	1.44	1.34
1	A	382[A]	TTS	OD1-CD1	3.86	1.34	1.24
1	B	382[B]	TTS	OD1-CD1	3.80	1.34	1.24
1	A	382[B]	TTS	OD1-CD1	3.78	1.34	1.24
1	B	382[B]	TTS	C5'-C6'	3.36	1.44	1.38
1	A	382[B]	TTS	C5'-C6'	3.32	1.44	1.38
1	B	382[B]	TTS	C2'-C3'	3.29	1.44	1.38
1	A	382[A]	TTS	C2'-C3'	3.25	1.44	1.38
1	B	382[A]	TTS	C2'-C3'	3.25	1.44	1.38
1	A	382[B]	TTS	C2'-C3'	3.20	1.44	1.38
1	B	382[B]	TTS	CG-CD1	-3.07	1.44	1.49
1	A	382[B]	TTS	CG-CD1	-3.06	1.44	1.49
1	B	382[A]	TTS	C5'-C6'	3.03	1.43	1.38
1	A	382[A]	TTS	C5'-C6'	3.02	1.43	1.38
1	B	382[A]	TTS	CG-CD1	-2.91	1.45	1.49
1	A	382[A]	TTS	CG-CD1	-2.89	1.45	1.49
1	A	382[B]	TTS	C2'-C1'	2.82	1.44	1.38
1	B	382[B]	TTS	C2'-C1'	2.82	1.44	1.38
1	A	382[A]	TTS	C2'-C1'	2.65	1.44	1.38
1	B	382[A]	TTS	C2'-C1'	2.64	1.44	1.38
1	B	382[A]	TTS	C6'-C1'	2.50	1.43	1.38
1	A	382[A]	TTS	C6'-C1'	2.50	1.43	1.38
1	B	382[B]	TTS	C6'-C1'	2.47	1.43	1.38
1	A	382[B]	TTS	C6'-C1'	2.45	1.43	1.38
1	B	382[A]	TTS	C3'-C4'	2.15	1.43	1.39
1	A	382[A]	TTS	C3'-C4'	2.14	1.43	1.39
1	B	382[B]	TTS	C3'-C4'	2.10	1.42	1.39
1	A	382[B]	TTS	C3'-C4'	2.08	1.42	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382[A]	TTS	CD2-CG-CD1	5.41	122.51	118.66
1	B	382[A]	TTS	CD2-CG-CD1	5.41	122.51	118.66
1	A	382[B]	TTS	CD2-CG-CD1	5.33	122.45	118.66
1	B	382[B]	TTS	CD2-CG-CD1	5.29	122.42	118.66
1	B	382[B]	TTS	CD2-CE2-CZ	3.18	121.04	117.44
1	A	382[B]	TTS	CD2-CE2-CZ	3.15	121.01	117.44
1	A	382[A]	TTS	CD2-CE2-CZ	3.09	120.94	117.44
1	B	382[A]	TTS	CD2-CE2-CZ	3.09	120.94	117.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382[A]	TTS	C1-NE2-CE2	2.90	127.64	121.36
1	B	382[A]	TTS	C1-NE2-CE2	2.90	127.64	121.36
1	A	382[B]	TTS	C1-NE2-CE2	2.82	127.47	121.36
1	B	382[B]	TTS	C1-NE2-CE2	2.81	127.44	121.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	382[A]	TTS	O-C-CA-CB
1	A	382[A]	TTS	NE2-C1-C2-C1'
1	A	382[B]	TTS	O-C-CA-CB
1	B	382[A]	TTS	O-C-CA-CB
1	B	382[A]	TTS	NE2-C1-C2-C1'
1	B	382[B]	TTS	O-C-CA-CB
1	A	382[A]	TTS	N-CA-CB-CG
1	B	382[A]	TTS	N-CA-CB-CG
1	A	382[B]	TTS	N-CA-CB-CG
1	B	382[B]	TTS	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	382[A]	TTS	4	0
1	A	382[B]	TTS	2	0
1	B	382[B]	TTS	2	0
1	A	382[A]	TTS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	382[A]:TTS	C	383:ASP	N	1.17
1	B	382[B]:TTS	C	383:ASP	N	1.14

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	619/638 (97%)	0.30	29 (4%)	36 44	20, 29, 45, 80	0
1	B	619/638 (97%)	0.13	24 (3%)	43 52	18, 26, 40, 79	0
All	All	1238/1276 (97%)	0.21	53 (4%)	40 49	18, 28, 43, 80	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	ALA	6.7
1	B	51	ALA	6.6
1	A	55	ALA	5.7
1	B	52	GLY	5.4
1	B	296	TYR	5.4
1	A	296	TYR	4.9
1	A	52	GLY	4.6
1	A	628	ASN	4.6
1	A	56	GLU	4.3
1	B	56	GLU	4.3
1	A	51	ALA	4.2
1	B	9	ALA	4.1
1	B	54	GLU	3.9
1	A	9	ALA	3.9
1	B	628	ASN	3.7
1	B	53	SER	3.7
1	B	50	GLY	3.5
1	B	414	GLY	3.4
1	A	54	GLU	3.2
1	A	148	ARG	3.1
1	A	267	ARG	2.9
1	A	68	SER	2.9
1	A	107	VAL	2.8
1	A	53	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	315	CYS	2.6
1	B	39	ILE	2.6
1	B	379	ILE	2.6
1	B	267	ARG	2.6
1	A	266	ASP	2.5
1	A	105	PHE	2.5
1	A	315	CYS	2.5
1	A	627	ALA	2.5
1	A	414	GLY	2.4
1	A	79	VAL	2.4
1	B	194	VAL	2.4
1	B	48	ALA	2.4
1	A	332	PHE	2.4
1	B	265	GLY	2.3
1	A	70	ALA	2.3
1	B	280	MET	2.2
1	B	314	GLY	2.2
1	A	209	LEU	2.2
1	B	220	ILE	2.2
1	A	85	ILE	2.2
1	B	419	ILE	2.2
1	A	143	GLU	2.1
1	A	321	ILE	2.1
1	A	507	ASN	2.1
1	A	338	ILE	2.1
1	B	266	ASP	2.1
1	A	260	ILE	2.1
1	A	328	ILE	2.1
1	B	321	ILE	2.1

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

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(Å ²)	Q<0.9
1	TTS	B	382[A]	23/24	0.76	0.22	27,44,56,56	23
1	TTS	B	382[B]	23/24	0.76	0.22	26,43,55,56	23
1	TTS	A	382[A]	23/24	0.85	0.18	25,44,57,58	23
1	TTS	A	382[B]	23/24	0.85	0.18	25,44,56,56	23

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	CU	A	1001	1/1	1.00	0.02	27,27,27,27	0
2	CU	B	1002	1/1	1.00	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.