



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:22 AM UTC

PDB ID : 7DKE / pdb_00007dke
Title : Stenotrophomonas maltophilia DPP7 in complex with Phe-Tyr
Authors : Sakamoto, Y.; Nakamura, A.; Suzuki, Y.; Honma, N.; Roppongi, S.; Kushibiki, C.; Yonezawa, N.; Takahashi, M.; Shida, Y.; Gouda, H.; Nonaka, T.; Ogasawara, W.; Tanaka, N.
Deposited on : 2020-11-23
Resolution : 1.91 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

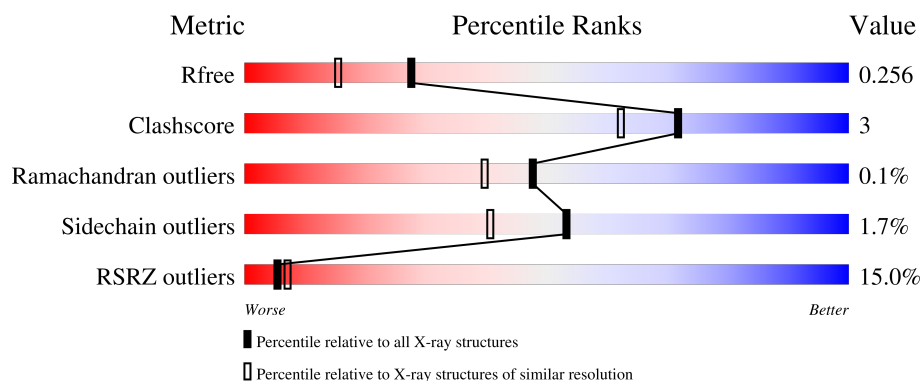
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	720	5% 89% 8% .
1	B	720	24% 85% 11% .

2 Entry composition [i](#)

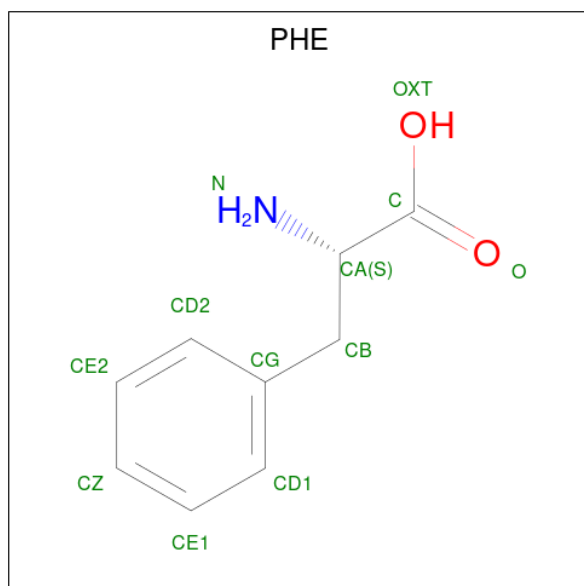
There are 5 unique types of molecules in this entry. The entry contains 11606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl-peptidase.

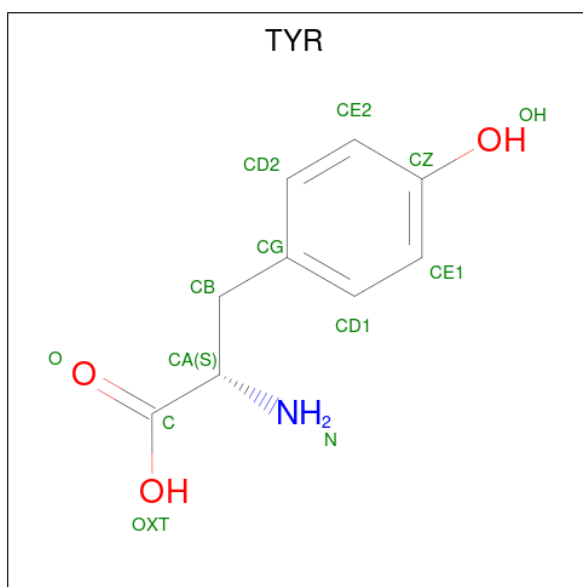
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	0	0
			5329	3375	927	1008	19			
1	B	697	Total	C	N	O	S	0	1	0
			5338	3380	928	1011	19			

- Molecule 2 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	B	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 3 is TYROSINE (CCD ID: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

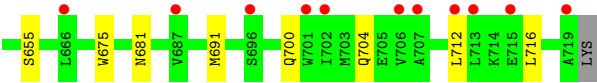
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	644	Total	O	0	0
			644	644		
5	B	217	Total	O	0	0
			217	217		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.03Å 74.56Å 153.87Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	40.00 – 1.91 40.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.91) 99.7 (40.00-1.91)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.251 0.214 , 0.256	Depositor DCC
R_{free} test set	5862 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11606	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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](#)

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

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	1.10	1/5442 (0.0%)	1.35	9/7375 (0.1%)
1	B	1.06	0/5451	1.46	5/7387 (0.1%)
All	All	1.08	1/10893 (0.0%)	1.41	14/14762 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	692	ILE	C-O	5.70	1.30	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ARG	CB-CA-C	-6.58	101.91	111.91
1	A	513	ARG	CG-CD-NE	-5.72	99.41	112.00
1	A	577	SER	CA-C-N	5.67	128.89	120.95
1	A	577	SER	C-N-CA	5.67	128.89	120.95
1	A	90	ILE	N-CA-C	-5.53	105.13	110.72
1	A	324	ALA	CA-C-O	-5.38	115.17	120.82
1	B	640	VAL	N-CA-C	-5.33	104.05	108.63
1	B	545	GLU	CA-C-N	5.27	125.95	119.99
1	B	545	GLU	C-N-CA	5.27	125.95	119.99
1	B	131	VAL	CA-C-N	5.20	127.51	120.65
1	B	131	VAL	C-N-CA	5.20	127.51	120.65
1	A	210	ASP	CA-CB-CG	-5.19	107.41	112.60
1	A	512	ASP	CA-C-N	5.14	127.43	120.38
1	A	512	ASP	C-N-CA	5.14	127.43	120.38

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	5329	0	5271	29	0
1	B	5338	0	5276	40	0
2	A	11	0	8	0	0
2	B	11	0	8	0	0
3	A	13	0	9	1	0
3	B	13	0	9	1	0
4	A	24	0	32	2	0
4	B	6	0	8	1	0
5	A	644	0	0	7	1
5	B	217	0	0	2	0
All	All	11606	0	10621	71	1

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 3.

All (71) 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)
4:A:806:GOL:H31	5:A:1203:HOH:O	1.55	1.06
1:A:334:LEU:HD12	5:A:1013:HOH:O	1.67	0.93
4:A:806:GOL:C3	5:A:1203:HOH:O	2.26	0.72
1:A:220:THR:H	1:A:643:ASN:HD21	1.41	0.65
1:B:275:ASN:HD22	1:B:681:ASN:ND2	1.96	0.63
1:B:700:GLN:HE21	1:B:704:GLN:NE2	1.96	0.63
1:B:275:ASN:HD22	1:B:681:ASN:HD21	1.47	0.62
1:B:655:SER:OG	3:B:802:TYR:C	2.42	0.62
1:B:189:MET:HE3	1:B:236:PRO:HD3	1.81	0.61
1:A:275:ASN:HD22	1:A:681:ASN:ND2	1.99	0.60
1:A:275:ASN:HD22	1:A:681:ASN:HD21	1.50	0.58
1:B:78:LEU:HD21	1:B:712:LEU:CD2	2.33	0.58
1:A:82:ASN:HD21	1:A:671:PHE:HA	1.69	0.58
1:B:136:LYS:O	1:B:139:ILE:HG13	2.04	0.57
1:A:655:SER:OG	3:A:802:TYR:C	2.47	0.57
1:B:552:ARG:HB3	1:B:553:PRO:HD3	1.87	0.56
1:A:232:LYS:NZ	1:A:242:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LEU:HG	1:B:44:LEU:HD22	1.89	0.54
1:B:172:CYS:HA	1:B:186:PHE:O	2.07	0.54
1:A:82:ASN:HD22	1:A:84:HIS:CE1	2.26	0.53
1:B:526:TYR:CZ	1:B:530:VAL:HG11	2.43	0.53
1:B:220:THR:H	1:B:643:ASN:HD21	1.56	0.52
1:A:215:MET:HE2	5:A:1240:HOH:O	2.11	0.51
1:B:216:TRP:CG	1:B:217:PRO:HA	2.46	0.51
1:A:267:VAL:HG13	1:A:657:SER:HB3	1.91	0.50
1:B:410:TYR:CE2	1:B:528:VAL:HA	2.46	0.50
1:A:410:TYR:CE2	1:A:528:VAL:HA	2.46	0.50
1:B:24:GLU:OE2	1:B:571:TYR:OH	2.16	0.50
1:B:324:ALA:HB1	4:B:803:GOL:H11	1.94	0.49
1:B:605:ALA:HB2	1:B:624:VAL:HG11	1.95	0.49
1:B:218:ARG:HB3	1:B:643:ASN:HD22	1.77	0.49
1:A:216:TRP:CG	1:A:217:PRO:HA	2.48	0.48
1:B:82:ASN:HD22	1:B:84:HIS:CE1	2.31	0.48
1:B:540:GLN:NE2	5:B:908:HOH:O	2.46	0.48
1:B:35:ILE:O	1:B:39:LEU:HB2	2.13	0.48
1:B:275:ASN:ND2	1:B:681:ASN:HD21	2.10	0.48
1:A:648:LEU:HD12	1:A:648:LEU:N	2.31	0.46
1:B:338[B]:GLU:CD	1:B:675:TRP:HE1	2.24	0.46
1:A:540:GLN:NE2	5:A:918:HOH:O	2.48	0.46
1:B:158:LYS:NZ	1:B:423:ARG:O	2.35	0.46
1:B:646:SER:OG	1:B:691:MET:HE2	2.16	0.45
1:A:368:LYS:N	1:A:369:PRO:CD	2.79	0.45
1:B:254:PHE:CE1	1:B:716:LEU:HD22	2.51	0.45
1:A:275:ASN:ND2	1:A:681:ASN:HD21	2.14	0.45
1:A:600:THR:HB	1:A:639:SER:HB3	1.99	0.45
1:B:145:ASP:O	1:B:146:PRO:C	2.60	0.44
1:A:646:SER:OG	1:A:691:MET:HE2	2.18	0.44
1:B:597:PRO:O	1:B:644:PHE:HA	2.17	0.43
1:B:82:ASN:HD22	1:B:655:SER:HB3	1.82	0.43
1:A:363:GLN:NE2	5:A:929:HOH:O	2.52	0.43
1:B:191:ILE:HG21	1:B:228:ALA:HB1	2.01	0.42
1:B:368:LYS:N	1:B:369:PRO:CD	2.83	0.42
1:B:301:VAL:CG1	1:B:326:MET:HE1	2.50	0.42
1:B:56:GLY:O	1:B:60:GLY:N	2.46	0.42
1:A:216:TRP:CD2	1:A:217:PRO:HA	2.54	0.42
1:A:299:ASN:HD22	1:A:299:ASN:HA	1.78	0.41
1:B:54:LEU:HD12	1:B:128:ILE:HD12	2.02	0.41
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ALA:HB2	1:A:156:PHE:CE2	2.55	0.41
1:B:341:LYS:NZ	5:B:904:HOH:O	2.38	0.41
1:A:125:LEU:HA	1:A:188:ASN:HD22	1.85	0.41
1:A:219:HIS:HB3	1:A:604:VAL:HG22	2.01	0.41
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.90	0.41
1:B:397:PHE:CE1	1:B:459:LEU:HD11	2.56	0.41
1:B:600:THR:HB	1:B:639:SER:HB3	2.02	0.41
1:A:406:ALA:HB2	1:A:499:LEU:CD1	2.51	0.41
1:B:216:TRP:CD2	1:B:217:PRO:HA	2.56	0.41
1:B:555:TYR:O	1:B:559:VAL:HG23	2.20	0.40
1:A:597:PRO:O	1:A:644:PHE:HA	2.21	0.40
1:B:575:ASN:O	1:B:576:LEU:HB2	2.21	0.40
1:A:45:LYS:HE2	5:A:1480:HOH:O	2.21	0.40

All (1) 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)
5:A:1006:HOH:O	5:A:1053:HOH:O[2_555]	2.11	0.09

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	695/720 (96%)	677 (97%)	18 (3%)	0	100	100
1	B	696/720 (97%)	667 (96%)	28 (4%)	1 (0%)	48	40
All	All	1391/1440 (97%)	1344 (97%)	46 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	SER

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	540/557 (97%)	535 (99%)	5 (1%)	70	67
1	B	541/557 (97%)	528 (98%)	13 (2%)	43	28
All	All	1081/1114 (97%)	1063 (98%)	18 (2%)	53	41

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ARG
1	A	380	HIS
1	A	381	LEU
1	A	384	SER
1	A	712	LEU
1	B	46	LEU
1	B	150	SER
1	B	181	ASN
1	B	371	LEU
1	B	380	HIS
1	B	399	ASN
1	B	524	ILE
1	B	536	LYS
1	B	548	SER
1	B	549	LEU
1	B	576	LEU
1	B	586	MET
1	B	635	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	82	ASN
1	A	93	ASN
1	A	213	ASN
1	A	275	ASN
1	A	284	ASN
1	A	299	ASN
1	A	328	ASN
1	A	540	GLN
1	A	584	ASN
1	A	643	ASN
1	A	654	ASN
1	A	681	ASN
1	B	40	GLN
1	B	82	ASN
1	B	213	ASN
1	B	299	ASN
1	B	328	ASN
1	B	336	GLN
1	B	348	GLN
1	B	453	GLN
1	B	469	GLN
1	B	557	GLN
1	B	566	GLN
1	B	584	ASN
1	B	643	ASN
1	B	681	ASN
1	B	704	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 ligands 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
4	GOL	A	806	-	5,5,5	0.25	0	5,5,5	0.62	0
2	PHE	A	801	3	10,11,12	0.40	0	8,13,15	0.42	0
4	GOL	A	804	-	5,5,5	0.21	0	5,5,5	0.61	0
3	TYR	B	802	2	12,13,13	0.52	0	13,17,17	0.44	0
4	GOL	A	805	-	5,5,5	0.13	0	5,5,5	0.29	0
4	GOL	B	803	-	5,5,5	0.12	0	5,5,5	0.12	0
2	PHE	B	801	3	10,11,12	0.85	0	8,13,15	0.42	0
4	GOL	A	803	-	5,5,5	0.18	0	5,5,5	0.30	0
3	TYR	A	802	2	12,13,13	0.71	1 (8%)	13,17,17	0.71	0

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
4	GOL	A	806	-	-	2/4/4/4	-
2	PHE	A	801	3	-	0/5/6/8	0/1/1/1
4	GOL	A	804	-	-	2/4/4/4	-
3	TYR	B	802	2	-	5/8/8/8	0/1/1/1
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
2	PHE	B	801	3	-	0/5/6/8	0/1/1/1
4	GOL	A	803	-	-	4/4/4/4	-
3	TYR	A	802	2	-	4/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	TYR	OXT-C	-2.20	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	GOL	C1-C2-C3-O3
4	A	806	GOL	O1-C1-C2-C3
4	A	803	GOL	O1-C1-C2-C3
4	A	804	GOL	O1-C1-C2-C3
4	A	805	GOL	O1-C1-C2-C3
4	B	803	GOL	O1-C1-C2-C3
4	A	803	GOL	O2-C2-C3-O3
4	A	804	GOL	O1-C1-C2-O2
4	A	806	GOL	O1-C1-C2-O2
4	A	805	GOL	O1-C1-C2-O2
4	A	803	GOL	O1-C1-C2-O2
4	B	803	GOL	O1-C1-C2-O2
3	B	802	TYR	CA-CB-CG-CD1
3	B	802	TYR	CA-CB-CG-CD2
3	A	802	TYR	CA-CB-CG-CD1
3	B	802	TYR	OXT-C-CA-CB
3	A	802	TYR	CA-CB-CG-CD2
3	B	802	TYR	O-C-CA-CB
3	A	802	TYR	OXT-C-CA-CB
3	A	802	TYR	O-C-CA-CB
3	B	802	TYR	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	806	GOL	2	0
3	B	802	TYR	1	0
4	B	803	GOL	1	0
3	A	802	TYR	1	0

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	697/720 (96%)	0.50	35 (5%) 34 38	14, 24, 43, 88	0
1	B	697/720 (96%)	1.44	174 (24%) 2 2	14, 42, 66, 111	1 (0%)
All	All	1394/1440 (96%)	0.97	209 (14%) 5 7	14, 32, 62, 111	1 (0%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	7.3
1	B	523	ALA	6.3
1	B	355	ALA	5.6
1	B	406	ALA	5.2
1	B	381	LEU	5.1
1	B	620	LEU	5.0
1	B	139	ILE	4.6
1	B	241	ALA	4.5
1	B	421	ALA	4.5
1	B	168	ALA	4.3
1	B	356	VAL	4.2
1	B	191	ILE	4.2
1	B	479	LEU	4.1
1	B	713	LEU	4.0
1	B	135	ALA	4.0
1	B	474	VAL	3.9
1	B	719	ALA	3.9
1	A	385	LYS	3.9
1	B	515	ALA	3.9
1	B	516	PHE	3.8
1	A	383	THR	3.7
1	B	94	SER	3.7
1	B	432	LEU	3.6
1	B	550	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	567	GLY	3.5
1	B	546	GLY	3.5
1	B	48	PRO	3.5
1	A	380	HIS	3.5
1	B	378	LEU	3.5
1	B	128	ILE	3.4
1	B	154	ASP	3.4
1	B	380	HIS	3.4
1	A	668	GLY	3.4
1	B	372	ALA	3.3
1	B	427	TYR	3.3
1	B	61	ALA	3.3
1	B	54	LEU	3.3
1	B	153	LEU	3.3
1	B	169	GLY	3.2
1	A	273	ARG	3.2
1	B	95	THR	3.2
1	B	140	ALA	3.1
1	B	359	TRP	3.1
1	B	68	CYS	3.1
1	B	172	CYS	3.1
1	B	229	TYR	3.1
1	B	534	LEU	3.1
1	B	514	ALA	3.1
1	B	549	LEU	3.0
1	B	508	TRP	3.0
1	B	379	LYS	3.0
1	B	626	ALA	3.0
1	B	360	LEU	3.0
1	A	474	VAL	3.0
1	B	706	VAL	3.0
1	B	166	ALA	3.0
1	B	161	VAL	2.9
1	A	145	ASP	2.9
1	B	410	TYR	2.9
1	A	386	SER	2.9
1	B	46	LEU	2.9
1	B	265	VAL	2.9
1	B	39	LEU	2.9
1	B	535	LEU	2.9
1	B	183	TYR	2.8
1	B	239	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	280	ALA	2.8
1	B	712	LEU	2.8
1	B	58	PRO	2.8
1	B	103	ASP	2.8
1	B	524	ILE	2.8
1	B	543	ILE	2.8
1	B	559	VAL	2.8
1	B	554	LEU	2.8
1	A	35	ILE	2.8
1	A	719	ALA	2.7
1	B	163	ALA	2.7
1	B	439	LEU	2.7
1	A	384	SER	2.7
1	B	30	GLN	2.7
1	B	377	LEU	2.7
1	B	244	VAL	2.7
1	B	142	ALA	2.7
1	B	533	ALA	2.7
1	B	551	ALA	2.7
1	B	245	PRO	2.7
1	A	484	ALA	2.6
1	B	138	ALA	2.6
1	A	478	TRP	2.6
1	A	485	ALA	2.6
1	B	402	ALA	2.6
1	B	526	TYR	2.6
1	A	462	TYR	2.6
1	A	371	LEU	2.6
1	B	556	LEU	2.6
1	B	621	LEU	2.6
1	B	367	GLY	2.6
1	B	624	VAL	2.6
1	B	707	ALA	2.6
1	B	38	PRO	2.5
1	B	371	LEU	2.5
1	B	414	ILE	2.5
1	B	375	ALA	2.5
1	B	174	LEU	2.5
1	B	702	ILE	2.5
1	B	155	ALA	2.5
1	B	358	ALA	2.5
1	B	527	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	44	LEU	2.5
1	B	601	LEU	2.5
1	B	50	GLN	2.5
1	B	131	VAL	2.5
1	B	622	ASP	2.5
1	B	177	PHE	2.4
1	B	357	LEU	2.4
1	B	409	LEU	2.4
1	B	489	SER	2.4
1	B	305	ILE	2.4
1	B	425	ALA	2.4
1	B	522	PRO	2.4
1	B	528	VAL	2.4
1	B	279	LEU	2.4
1	B	334	LEU	2.4
1	A	210	ASP	2.4
1	A	523	ALA	2.4
1	B	36	ALA	2.4
1	B	162	ALA	2.4
1	B	127	GLN	2.4
1	B	181	ASN	2.4
1	B	696	SER	2.4
1	B	185	LEU	2.4
1	B	486	ALA	2.4
1	B	51	LEU	2.3
1	B	490	LEU	2.3
1	B	632	LEU	2.3
1	B	383	THR	2.3
1	B	426	GLY	2.3
1	B	582	PHE	2.3
1	A	365	ALA	2.3
1	B	560	ALA	2.3
1	A	294	ILE	2.3
1	B	386	SER	2.3
1	A	718	LEU	2.3
1	B	369	PRO	2.3
1	B	35	ILE	2.3
1	B	98	LYS	2.3
1	B	129	THR	2.3
1	B	147	LEU	2.3
1	B	666	LEU	2.3
1	B	173	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	673	GLY	2.2
1	B	56	GLY	2.2
1	B	170	PHE	2.2
1	B	226	TYR	2.2
1	B	365	ALA	2.2
1	B	511	ALA	2.2
1	B	555	TYR	2.2
1	B	63	VAL	2.2
1	A	377	LEU	2.2
1	B	125	LEU	2.2
1	B	475	LEU	2.2
1	B	612	ASP	2.2
1	B	629	TYR	2.2
1	B	715	GLU	2.2
1	A	68	CYS	2.2
1	A	378	LEU	2.2
1	B	499	LEU	2.2
1	A	143	GLY	2.2
1	B	618	LYS	2.2
1	B	34	GLU	2.2
1	B	282	GLU	2.2
1	B	420	ASP	2.2
1	A	357	LEU	2.2
1	A	535	LEU	2.2
1	B	100	LEU	2.2
1	B	518	ALA	2.2
1	B	444	ARG	2.2
1	B	53	ASN	2.1
1	B	343	ILE	2.1
1	B	40	GLN	2.1
1	B	701	TRP	2.1
1	B	196	LEU	2.1
1	B	353	GLU	2.1
1	B	366	ALA	2.1
1	B	623	ALA	2.1
1	B	313	ALA	2.1
1	B	540	GLN	2.1
1	B	273	ARG	2.1
1	B	401	SER	2.1
1	A	473	GLU	2.1
1	A	550	THR	2.1
1	B	143	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	2.1
1	B	197	VAL	2.1
1	B	376	GLN	2.1
1	B	576	LEU	2.1
1	A	527	ALA	2.1
1	B	149	ARG	2.1
1	B	111	LYS	2.0
1	B	176	SER	2.0
1	B	384	SER	2.0
1	B	407	ILE	2.0
1	B	610	GLY	2.0
1	B	75	PRO	2.0
1	B	394	VAL	2.0
1	B	687	VAL	2.0
1	A	151	ARG	2.0
1	B	346	ALA	2.0
1	A	489	SER	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(Å ²)	Q<0.9
4	GOL	A	803	6/6	0.76	0.16	36,44,46,48	0
4	GOL	A	805	6/6	0.82	0.12	26,34,37,38	0
4	GOL	A	806	6/6	0.83	0.14	29,37,41,43	0
3	TYR	B	802	13/13	0.84	0.11	23,25,30,31	0
4	GOL	B	803	6/6	0.85	0.12	40,42,45,47	0
4	GOL	A	804	6/6	0.86	0.13	30,37,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PHE	B	801	11/12	0.89	0.11	23,27,30,31	0
2	PHE	A	801	11/12	0.93	0.08	19,20,22,22	0
3	TYR	A	802	13/13	0.93	0.08	17,19,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.