



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2021 – 12:10 PM JST

PDB ID : 7DKD  
Title : Stenotrophomonas maltophilia DPP7 in complex with Asn-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 : 1.92 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

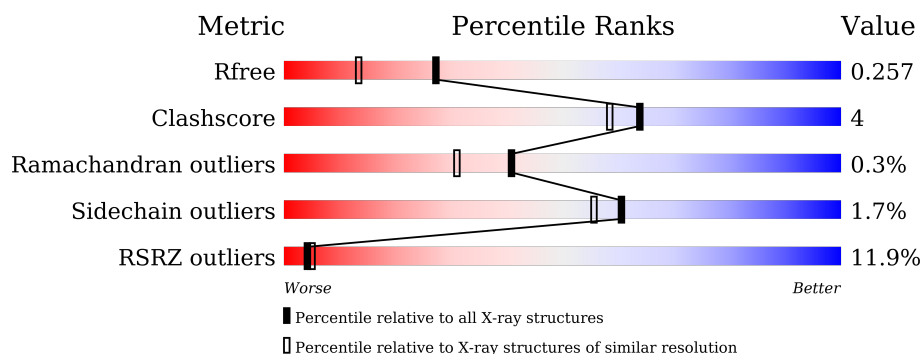
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	B	720	<div> <div style="width: 22%; height: 10px; background-color: red;"></div> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>

## 2 Entry composition [i](#)

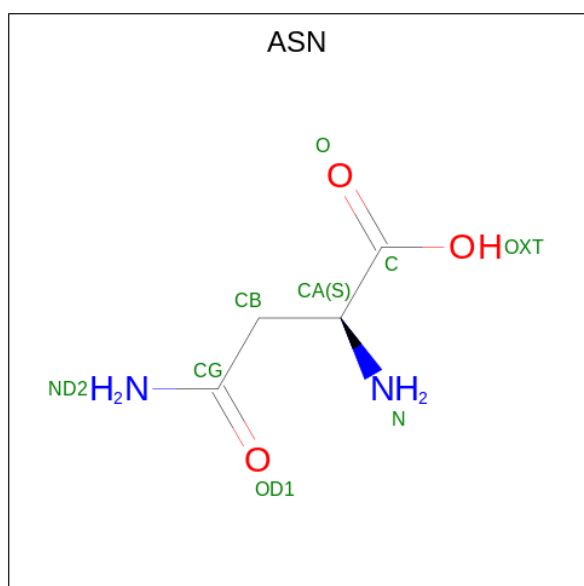
There are 5 unique types of molecules in this entry. The entry contains 11889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

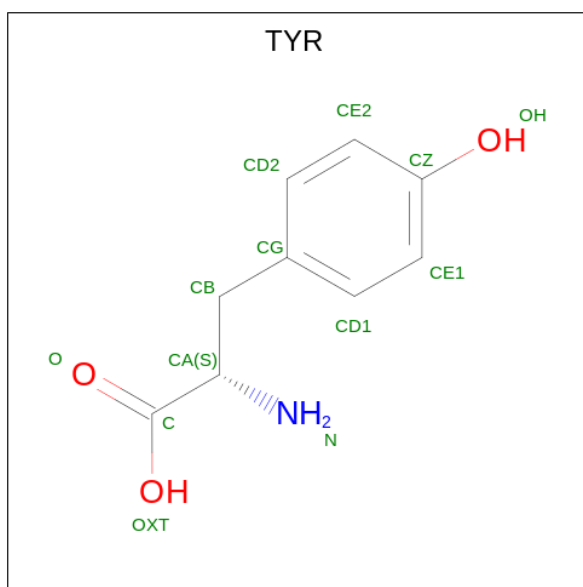
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	0	0
			5329	3375	927	1008	19			
1	B	697	Total	C	N	O	S	0	1	0
			5338	3380	928	1011	19			

- Molecule 2 is ASPARAGINE (three-letter code: ASN) (formula:  $C_4H_8N_2O_3$ ).



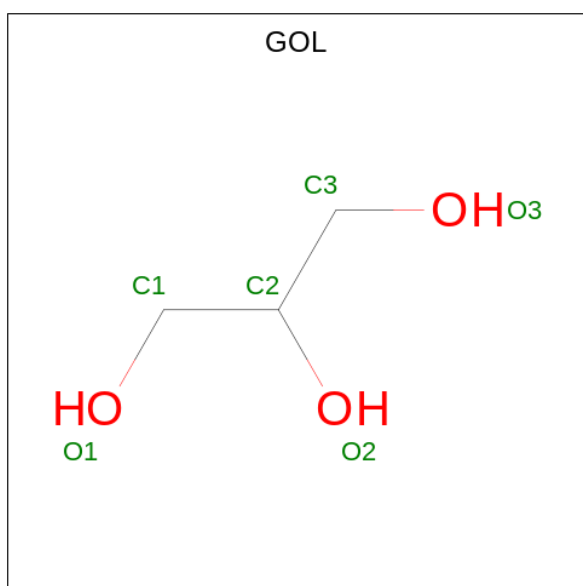
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	2	2		
2	B	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 3 is TYROSINE (three-letter code: 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 (three-letter code: 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		

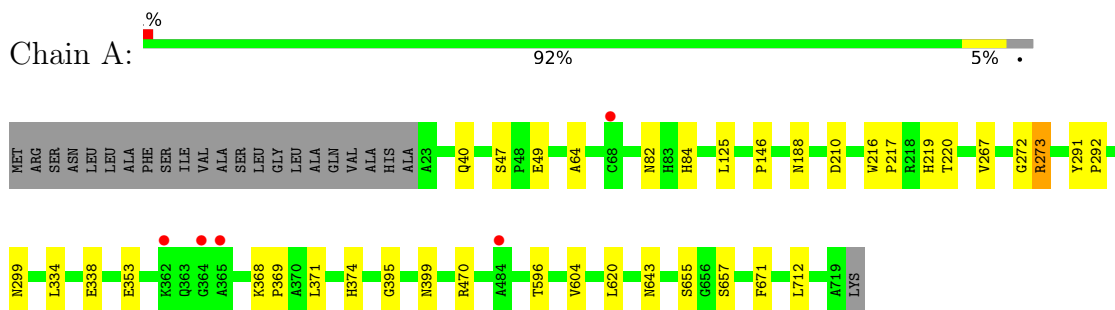
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	929	Total	O	0	0
			929	929		
5	B	233	Total	O	0	0
			233	233		

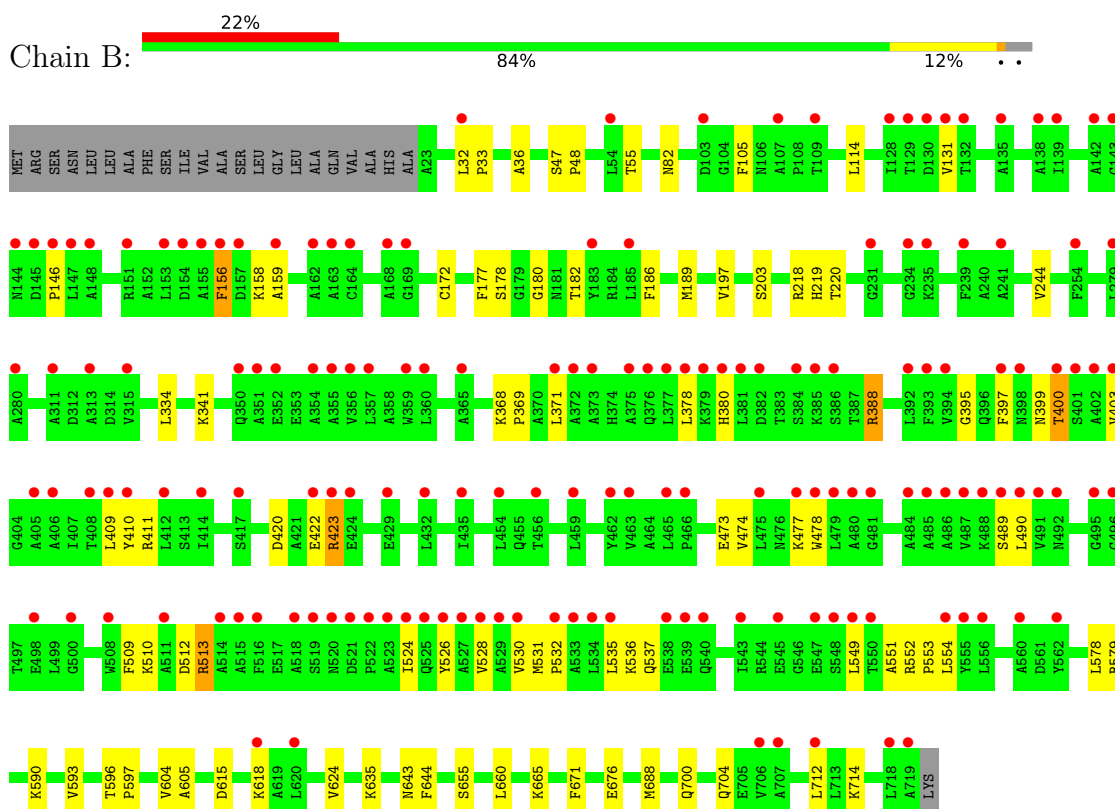
### 3 Residue-property plots [i](#)

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: Dipeptidyl-peptidase



#### • Molecule 1: Dipeptidyl-peptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.55Å 74.89Å 154.65Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	40.00 – 1.92 50.48 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.92) 99.6 (50.48-1.92)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.202 , 0.248 0.209 , 0.257	Depositor DCC
$R_{free}$ test set	6098 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.74	0/5442	0.86	0/7375
1	B	0.71	0/5451	0.81	0/7387
All	All	0.72	0/10893	0.83	0/14762

There are no bond length outliers.

There are no bond angle outliers.

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	30	0
1	B	5338	0	5276	57	0
2	A	8	0	5	0	0
2	B	8	0	5	0	0
3	A	13	0	9	1	0
3	B	13	0	9	1	0
4	A	18	0	24	3	0
5	A	929	0	0	11	0
5	B	233	0	0	12	0
All	All	11889	0	10599	89	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 4.

All (89) 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:334:LEU:HD21	5:B:1105:HOH:O	1.39	1.19
1:B:409:LEU:HA	5:B:1079:HOH:O	1.76	0.83
1:A:334:LEU:HD12	5:A:1164:HOH:O	1.79	0.82
1:B:47:SER:HB3	5:B:1051:HOH:O	1.80	0.81
1:B:409:LEU:HD23	5:B:1079:HOH:O	1.85	0.75
1:A:338:GLU:OE1	5:A:901:HOH:O	2.08	0.72
1:B:596:THR:HG21	5:B:995:HOH:O	1.89	0.72
1:B:220:THR:H	1:B:643:ASN:HD21	1.41	0.67
4:A:804:GOL:H31	5:A:1495:HOH:O	1.98	0.64
1:B:531:MET:HE3	1:B:535:LEU:HG	1.80	0.63
1:B:244:VAL:HG12	5:B:951:HOH:O	1.98	0.63
1:B:197:VAL:HG11	1:B:712:LEU:HD21	1.80	0.62
1:A:220:THR:H	1:A:643:ASN:HD21	1.47	0.62
1:B:474:VAL:O	1:B:478:TRP:HD1	1.84	0.61
1:B:397:PHE:O	1:B:400:THR:HB	2.03	0.59
4:A:804:GOL:C3	5:A:1495:HOH:O	2.51	0.58
1:B:590:LYS:HG2	1:B:593:VAL:CG1	2.33	0.58
1:B:189:MET:HB2	5:B:943:HOH:O	2.04	0.57
1:B:400:THR:HG22	1:B:403:VAL:HB	1.87	0.56
1:A:470:ARG:O	1:A:470:ARG:HG3	2.06	0.55
1:B:700:GLN:HE21	1:B:704:GLN:NE2	2.05	0.55
1:B:189:MET:CB	5:B:943:HOH:O	2.55	0.55
1:A:146:PRO:HD2	5:A:913:HOH:O	2.05	0.55
1:B:512:ASP:O	1:B:513:ARG:HB2	2.07	0.55
1:A:210:ASP:OD2	5:A:902:HOH:O	2.18	0.53
1:B:509:PHE:CE2	1:B:510:LYS:HE3	2.44	0.53
1:A:125:LEU:HA	1:A:188:ASN:HD22	1.72	0.52
1:B:526:TYR:CZ	1:B:530:VAL:HG11	2.45	0.52
1:B:32:LEU:N	1:B:33:PRO:CD	2.73	0.52
1:B:474:VAL:O	1:B:478:TRP:CD1	2.63	0.51
1:B:131:VAL:O	1:B:131:VAL:HG12	2.10	0.51
1:B:172:CYS:HA	1:B:186:PHE:O	2.11	0.51
1:A:655:SER:OG	3:A:802:TYR:C	2.49	0.51
1:B:605:ALA:HB2	1:B:624:VAL:HG11	1.92	0.50
1:B:474:VAL:O	1:B:477:LYS:HB3	2.12	0.50
1:B:552:ARG:HB3	1:B:553:PRO:HD3	1.92	0.50
1:A:272:GLY:O	1:A:273:ARG:HD3	2.11	0.49
1:B:655:SER:OG	3:B:802:TYR:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LEU:O	1:B:579:ARG:HD3	2.11	0.49
1:B:105:PHE:CZ	1:B:114:LEU:HG	2.47	0.49
1:B:410:TYR:CE2	1:B:528:VAL:HA	2.48	0.49
1:B:411:ARG:HD3	1:B:531:MET:HE1	1.95	0.49
1:A:64:ALA:HB1	4:A:803:GOL:H32	1.94	0.48
1:B:47:SER:CB	5:B:1051:HOH:O	2.50	0.47
1:B:714:LYS:NZ	5:B:908:HOH:O	2.47	0.47
1:B:551:ALA:O	1:B:554:LEU:HB2	2.15	0.46
1:B:218:ARG:HB3	1:B:643:ASN:HD22	1.80	0.46
1:A:267:VAL:HG13	1:A:657:SER:HB3	1.98	0.46
1:B:156:PHE:C	1:B:156:PHE:CD1	2.88	0.45
1:B:531:MET:N	1:B:532:PRO:CD	2.79	0.45
1:B:203:SER:HB2	1:B:615:ASP:O	2.17	0.45
1:B:219:HIS:HB3	1:B:604:VAL:HG22	1.98	0.45
1:B:158:LYS:NZ	1:B:423:ARG:O	2.48	0.45
1:B:388:ARG:HD2	5:B:1021:HOH:O	2.17	0.45
1:B:395:GLY:O	1:B:399:ASN:ND2	2.48	0.45
1:A:299:ASN:ND2	5:A:912:HOH:O	2.42	0.44
1:B:512:ASP:O	1:B:513:ARG:CB	2.65	0.44
1:B:597:PRO:O	1:B:644:PHE:HA	2.17	0.44
1:A:216:TRP:CG	1:A:217:PRO:HA	2.52	0.44
1:A:353:GLU:OE2	1:A:374:HIS:HE1	2.00	0.44
1:A:470:ARG:NH2	5:A:938:HOH:O	2.51	0.44
1:A:470:ARG:O	1:A:470:ARG:CG	2.66	0.43
1:B:159:ALA:HB3	5:B:917:HOH:O	2.17	0.43
1:A:82:ASN:HD22	1:A:655:SER:HB3	1.84	0.43
1:A:219:HIS:HB3	1:A:604:VAL:HG22	2.01	0.43
1:B:368:LYS:N	1:B:369:PRO:CD	2.82	0.43
1:A:395:GLY:O	1:A:399:ASN:ND2	2.48	0.43
1:B:177:PHE:O	1:B:180:GLY:N	2.48	0.43
1:A:82:ASN:HD21	1:A:671:PHE:HA	1.83	0.43
1:A:40:GLN:CG	5:A:1099:HOH:O	2.67	0.42
1:B:524:ILE:O	1:B:528:VAL:HG23	2.19	0.42
1:A:291:TYR:N	1:A:292:PRO:HD2	2.34	0.42
1:B:177:PHE:HB2	1:B:182:THR:HB	2.01	0.42
1:B:36:ALA:HB1	1:B:48:PRO:HG2	2.00	0.42
1:B:82:ASN:HD21	1:B:671:PHE:HA	1.85	0.42
1:A:40:GLN:HG3	5:A:1099:HOH:O	2.19	0.42
1:A:620:LEU:HD23	1:A:620:LEU:C	2.40	0.42
1:A:596:THR:HG21	5:A:1334:HOH:O	2.20	0.41
1:A:82:ASN:HD22	1:A:84:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.93	0.41
1:B:341:LYS:HA	1:B:341:LYS:HD3	1.90	0.41
1:B:197:VAL:CG1	1:B:712:LEU:HD21	2.48	0.41
1:B:420:ASP:C	1:B:422:GLU:H	2.24	0.41
1:B:676:GLU:HG2	1:B:688:MET:CE	2.51	0.41
1:A:368:LYS:N	1:A:369:PRO:CD	2.84	0.41
1:A:220:THR:H	1:A:643:ASN:ND2	2.16	0.40
1:A:82:ASN:ND2	1:A:655:SER:HB3	2.37	0.40
1:B:490:LEU:HD12	1:B:490:LEU:O	2.20	0.40
1:B:660:LEU:HA	1:B:665:LYS:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	695/720 (96%)	676 (97%)	19 (3%)	0	100	100
1	B	696/720 (97%)	643 (92%)	49 (7%)	4 (1%)	25	14
All	All	1391/1440 (97%)	1319 (95%)	68 (5%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	SER
1	B	513	ARG
1	B	473	GLU
1	B	146	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	540/557 (97%)	536 (99%)	4 (1%)	84	83
1	B	541/557 (97%)	527 (97%)	14 (3%)	46	37
All	All	1081/1114 (97%)	1063 (98%)	18 (2%)	60	55

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

Mol	Chain	Res	Type
1	A	47	SER
1	A	49	GLU
1	A	273	ARG
1	A	712	LEU
1	B	55	THR
1	B	156	PHE
1	B	371	LEU
1	B	378	LEU
1	B	380	HIS
1	B	388	ARG
1	B	400	THR
1	B	423	ARG
1	B	489	SER
1	B	536	LYS
1	B	537	GLN
1	B	549	LEU
1	B	618	LYS
1	B	635	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	144	ASN
1	A	188	ASN
1	A	350	GLN

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Mol	Chain	Res	Type
1	A	374	HIS
1	A	540	GLN
1	A	584	ASN
1	A	643	ASN
1	A	654	ASN
1	B	50	GLN
1	B	82	ASN
1	B	275	ASN
1	B	374	HIS
1	B	520	ASN
1	B	584	ASN
1	B	643	ASN
1	B	681	ASN
1	B	704	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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	805	-	5,5,5	0.15	0	5,5,5	0.32	0
4	GOL	A	804	-	5,5,5	0.24	0	5,5,5	0.43	0
3	TYR	B	802	2	10,13,13	0.31	0	12,17,17	0.79	1 (8%)
3	TYR	A	802	2	10,13,13	0.28	0	12,17,17	0.69	0
2	ASN	A	801	3	6,7,8	0.84	0	5,8,10	0.66	0
2	ASN	B	801	3	6,7,8	0.84	0	5,8,10	0.51	0
4	GOL	A	803	-	5,5,5	0.24	0	5,5,5	0.59	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	805	-	-	4/4/4/4	-
4	GOL	A	804	-	-	1/4/4/4	-
3	TYR	B	802	2	-	4/4/8/8	0/1/1/1
3	TYR	A	802	2	-	3/4/8/8	0/1/1/1
2	ASN	A	801	3	-	0/5/6/8	-
2	ASN	B	801	3	-	0/5/6/8	-
4	GOL	A	803	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	TYR	CB-CA-C	2.58	114.86	110.69

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	A	804	GOL	O1-C1-C2-O2
3	A	802	TYR	CA-CB-CG-CD1
3	B	802	TYR	CA-CB-CG-CD2
3	A	802	TYR	N-CA-CB-CG
4	A	805	GOL	O2-C2-C3-O3
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	804	GOL	2	0
3	B	802	TYR	1	0
3	A	802	TYR	1	0
4	A	803	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	697/720 (96%)	0.01	5 (0%) <span>87</span> <span>89</span>	6, 15, 35, 73	0
1	B	697/720 (96%)	1.24	161 (23%) <span>0</span> <span>0</span>	11, 45, 78, 105	0
All	All	1394/1440 (96%)	0.62	166 (11%) <span>4</span> <span>5</span>	6, 26, 71, 105	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	479	LEU	7.3
1	B	526	TYR	7.2
1	B	534	LEU	6.8
1	B	381	LEU	6.7
1	B	719	ALA	6.6
1	B	378	LEU	6.3
1	B	159	ALA	6.2
1	B	142	ALA	6.0
1	B	484	ALA	5.8
1	B	410	TYR	5.6
1	B	491	VAL	5.6
1	B	535	LEU	5.5
1	B	406	ALA	5.4
1	B	139	ILE	5.2
1	B	548	SER	5.2
1	B	402	ALA	4.9
1	B	475	LEU	4.9
1	B	523	ALA	4.9
1	B	376	GLN	4.7
1	B	168	ALA	4.5
1	B	478	TRP	4.4
1	B	146	PRO	4.4
1	B	515	ALA	4.3
1	B	385	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	516	PHE	4.2
1	B	432	LEU	4.2
1	B	380	HIS	4.2
1	B	529	ALA	4.2
1	B	144	ASN	4.2
1	B	496	GLY	4.1
1	B	488	LYS	4.1
1	B	487	VAL	4.1
1	B	356	VAL	4.0
1	B	481	GLY	3.9
1	B	135	ALA	3.9
1	B	485	ALA	3.9
1	B	143	GLY	3.9
1	B	508	TRP	3.8
1	B	409	LEU	3.8
1	B	375	ALA	3.7
1	B	554	LEU	3.7
1	B	511	ALA	3.6
1	B	377	LEU	3.6
1	B	423	ARG	3.6
1	B	414	ILE	3.6
1	B	360	LEU	3.5
1	B	540	GLN	3.5
1	B	379	LYS	3.5
1	B	417	SER	3.5
1	B	393	PHE	3.5
1	B	412	LEU	3.4
1	B	164	CYS	3.4
1	B	351	ALA	3.3
1	B	620	LEU	3.3
1	B	147	LEU	3.3
1	B	128	ILE	3.3
1	B	231	GLY	3.3
1	B	489	SER	3.3
1	B	372	ALA	3.3
1	B	518	ALA	3.3
1	B	525	GLN	3.3
1	B	463	VAL	3.2
1	B	543	ILE	3.2
1	B	169	GLY	3.2
1	B	718	LEU	3.2
1	B	547	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	162	ALA	3.2
1	B	530	VAL	3.2
1	B	384	SER	3.2
1	B	145	ASP	3.1
1	B	532	PRO	3.1
1	B	492	ASN	3.1
1	B	522	PRO	3.1
1	B	405	ALA	3.1
1	B	435	ILE	3.0
1	B	32	LEU	3.0
1	B	533	ALA	3.0
1	B	397	PHE	3.0
1	B	365	ALA	3.0
1	B	514	ALA	2.9
1	B	355	ALA	2.9
1	B	459	LEU	2.9
1	B	354	ALA	2.9
1	B	712	LEU	2.9
1	B	424	GLU	2.8
1	B	524	ILE	2.8
1	B	386	SER	2.8
1	B	138	ALA	2.8
1	B	618	LYS	2.8
1	B	153	LEU	2.7
1	B	371	LEU	2.7
1	B	155	ALA	2.7
1	B	156	PHE	2.7
1	B	490	LEU	2.7
1	B	545	GLU	2.7
1	B	398	ASN	2.7
1	B	241	ALA	2.6
1	B	313	ALA	2.6
1	B	707	ALA	2.6
1	B	528	VAL	2.6
1	B	539	GLU	2.6
1	B	373	ALA	2.6
1	B	280	ALA	2.6
1	B	311	ALA	2.6
1	B	154	ASP	2.6
1	B	550	THR	2.6
1	B	357	LEU	2.6
1	A	484	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	163	ALA	2.6
1	B	352	GLU	2.6
1	B	555	TYR	2.5
1	B	520	ASN	2.5
1	B	477	LYS	2.5
1	A	365	ALA	2.4
1	B	130	ASP	2.4
1	B	239	PHE	2.4
1	B	350	GLN	2.4
1	B	234	GLY	2.4
1	B	400	THR	2.4
1	B	279	LEU	2.4
1	B	500	GLY	2.4
1	B	480	ALA	2.4
1	B	466	PRO	2.4
1	B	465	LEU	2.4
1	B	107	ALA	2.4
1	B	382	ASP	2.4
1	B	394	VAL	2.4
1	B	519	SER	2.4
1	B	359	TRP	2.3
1	B	556	LEU	2.3
1	B	706	VAL	2.3
1	B	498	GLU	2.3
1	B	254	PHE	2.3
1	B	235	LYS	2.3
1	B	103	ASP	2.3
1	B	454	LEU	2.3
1	B	132	THR	2.3
1	B	422	GLU	2.3
1	B	131	VAL	2.2
1	B	129	THR	2.2
1	B	408	THR	2.2
1	B	429	GLU	2.2
1	B	148	ALA	2.2
1	B	392	LEU	2.2
1	B	109	THR	2.2
1	B	521	ASP	2.2
1	B	54	LEU	2.2
1	B	456	THR	2.2
1	B	562	TYR	2.2
1	B	538	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	527	ALA	2.1
1	B	560	ALA	2.1
1	B	315	VAL	2.1
1	B	549	LEU	2.1
1	B	183	TYR	2.1
1	B	495	GLY	2.1
1	A	362	LYS	2.1
1	B	401	SER	2.1
1	B	486	ALA	2.1
1	B	157	ASP	2.1
1	B	151	ARG	2.0
1	B	403	VAL	2.0
1	A	364	GLY	2.0
1	A	68	CYS	2.0
1	B	462	TYR	2.0
1	B	185	LEU	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 monosaccharides 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, 95<sup>th</sup> 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
4	GOL	A	804	6/6	0.86	0.18	18,25,27,28	0
3	TYR	B	802	13/13	0.87	0.14	21,25,28,34	0
4	GOL	A	805	6/6	0.87	0.24	32,38,41,42	0
4	GOL	A	803	6/6	0.90	0.15	23,28,29,30	0
2	ASN	B	801	8/9	0.93	0.12	23,24,28,31	0
3	TYR	A	802	13/13	0.94	0.13	13,16,18,23	0
2	ASN	A	801	8/9	0.95	0.12	11,13,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.