



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2021 – 12:10 PM JST

PDB ID : 7DKE  
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](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

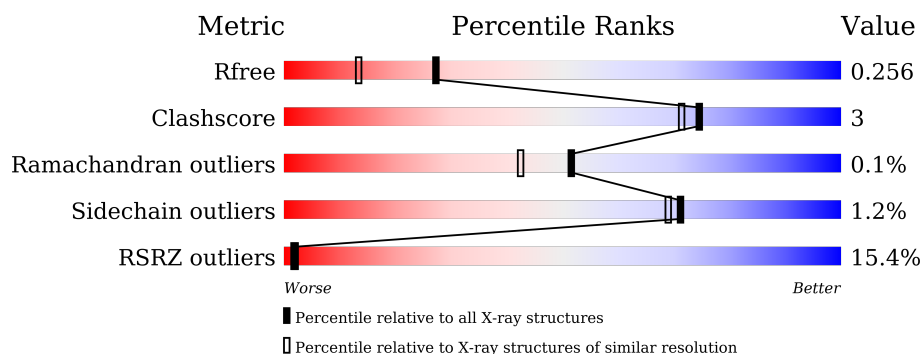
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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))
$R_{free}$	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>6%</div> <div>90%</div> <div>6%</div> </div>
1	B	720	<div> <div>24%</div> <div>87%</div> <div>9%</div> </div>

## 2 Entry composition [i](#)

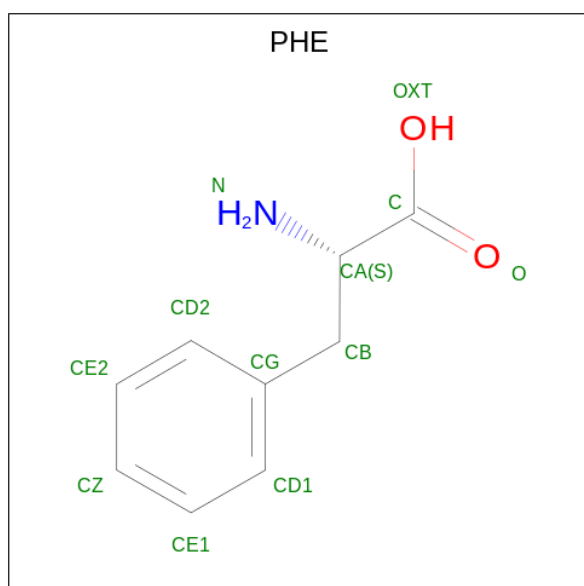
There are 5 unique types of molecules in this entry. The entry contains 11606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

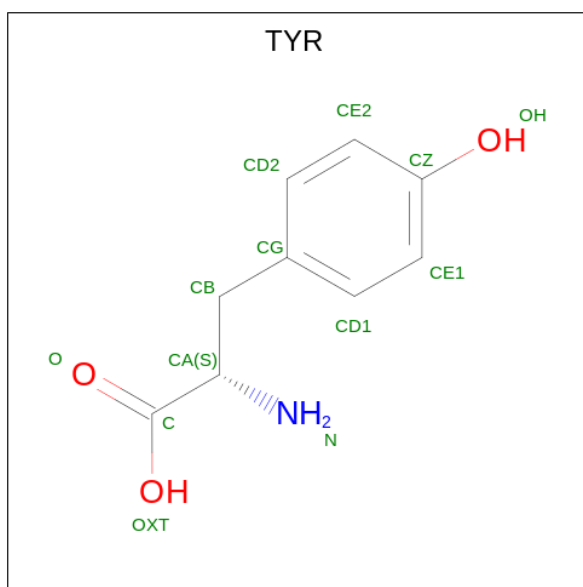
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	0	0
			5329	3375	927	1008	19			
1	B	697	Total	C	N	O	S	0	1	0
			5338	3380	928	1011	19			

- Molecule 2 is PHENYLALANINE (three-letter code: PHE) (formula:  $C_9H_{11}NO_2$ ).



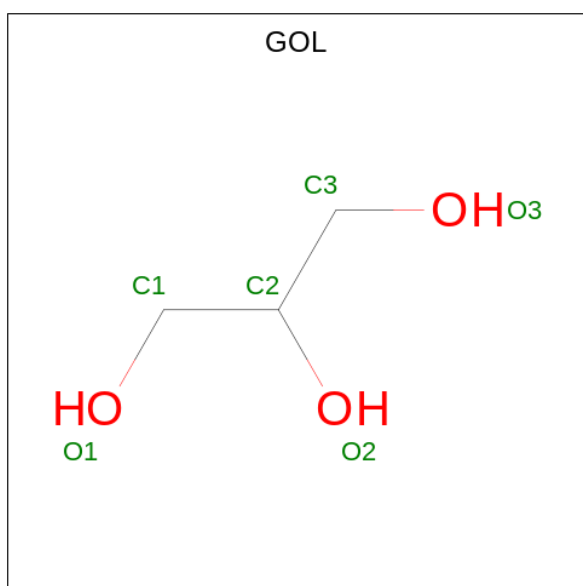
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	B	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 3 is TYROSINE (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		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

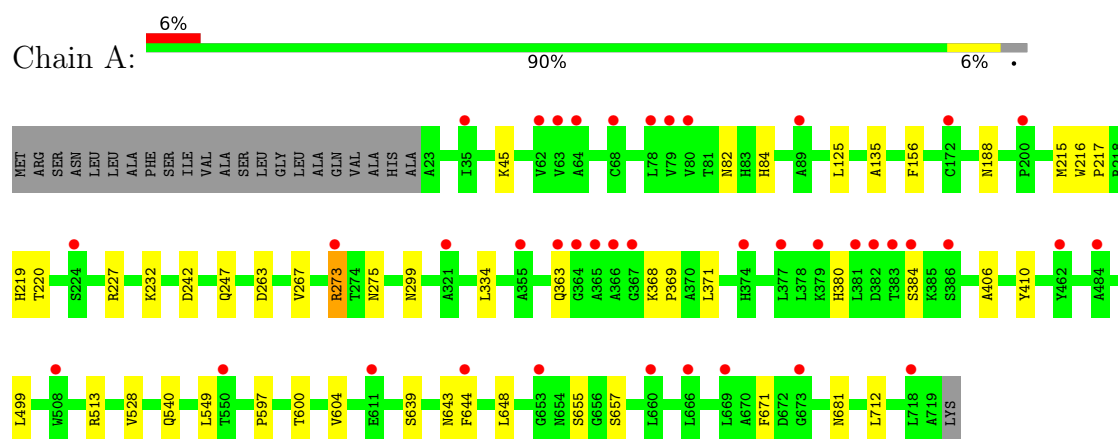
- Molecule 5 is water.

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

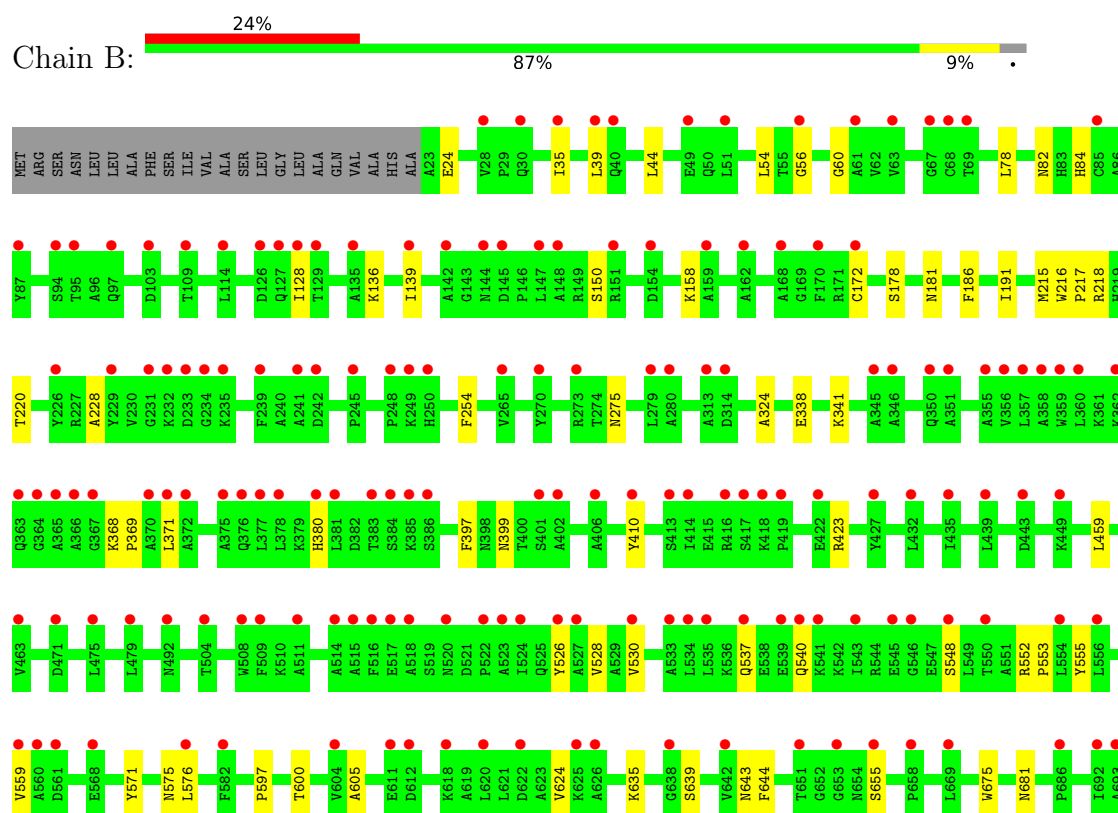
### 3 Residue-property plots [i](#)

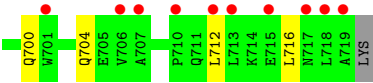
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, $\alpha$ , $\beta$ , $\gamma$	68.03Å 74.56Å 153.87Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	40.00 – 1.91 39.39 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.91) 99.7 (39.39-1.91)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<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 [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	0.75	0/5442	0.88	4/7375 (0.1%)
1	B	0.71	0/5451	0.82	0/7387
All	All	0.73	0/10893	0.85	4/14762 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ARG	NE-CZ-NH2	-10.23	115.18	120.30
1	A	273	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	513	ARG	CG-CD-NE	-5.90	99.41	111.80
1	A	227	ARG	NE-CZ-NH1	5.26	122.93	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	37	0
2	A	11	0	8	0	0
2	B	11	0	8	0	0
3	A	13	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	9	1	0
4	A	24	0	32	3	0
4	B	6	0	8	1	0
5	A	644	0	0	7	1
5	B	217	0	0	3	0
All	All	11606	0	10621	69	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 (69) 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: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:655:SER:OG	3:B:802:TYR:C	2.42	0.57
1:B:136:LYS:O	1:B:139:ILE:HG13	2.04	0.57
1:B:341:LYS:NZ	5:B:904:HOH:O	2.38	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
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:A:655:SER:OG	3:A:802:TYR:C	2.47	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:655:SER:HG	3:A:802:TYR:C	2.19	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: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:263:ASP:OD1	4:A:805:GOL:O1	2.31	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:215:MET:HE3	5:B:902:HOH:O	2.19	0.42
1:B:368:LYS:N	1:B:369:PRO:CD	2.83	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
1:A:135:ALA:HB2	1:A:156:PHE:CE2	2.55	0.41
1:B:338[B]:GLU:CD	1:B:675:TRP:HE1	2.24	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%)	51	42
All	All	1391/1440 (97%)	1344 (97%)	46 (3%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	SER

### 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	540/557 (97%)	535 (99%)	5 (1%)	78	78
1	B	541/557 (97%)	533 (98%)	8 (2%)	65	61
All	All	1081/1114 (97%)	1068 (99%)	13 (1%)	71	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	A	273	ARG
1	A	380	HIS
1	A	384	SER
1	A	712	LEU
1	B	150	SER
1	B	181	ASN
1	B	371	LEU
1	B	380	HIS
1	B	399	ASN
1	B	537	GLN
1	B	548	SER
1	B	635	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	82	ASN
1	A	284	ASN
1	A	332	ASN
1	A	336	GLN
1	A	348	GLN
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	91	GLN
1	B	213	ASN
1	B	299	ASN
1	B	328	ASN
1	B	348	GLN
1	B	453	GLN
1	B	557	GLN
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 monosaccharides 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	$\# Z  > 2$
2	PHE	B	801	3	10,11,12	0.79	0	10,13,15	0.54	0
4	GOL	A	804	-	5,5,5	0.21	0	5,5,5	0.59	0
4	GOL	A	803	-	5,5,5	0.17	0	5,5,5	0.29	0
2	PHE	A	801	3	10,11,12	0.35	0	10,13,15	0.80	1 (10%)
4	GOL	A	805	-	5,5,5	0.13	0	5,5,5	0.29	0
3	TYR	A	802	2	10,13,13	0.24	0	12,17,17	0.81	1 (8%)
3	TYR	B	802	2	10,13,13	0.39	0	12,17,17	0.66	0
4	GOL	A	806	-	5,5,5	0.23	0	5,5,5	0.58	0
4	GOL	B	803	-	5,5,5	0.11	0	5,5,5	0.13	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
2	PHE	B	801	3	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	804	-	-	2/4/4/4	-
4	GOL	A	803	-	-	4/4/4/4	-
2	PHE	A	801	3	-	0/5/6/8	0/1/1/1
4	GOL	A	805	-	-	2/4/4/4	-
3	TYR	A	802	2	-	2/4/8/8	0/1/1/1
3	TYR	B	802	2	-	2/4/8/8	0/1/1/1
4	GOL	A	806	-	-	2/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	TYR	CB-CA-C	2.28	114.38	110.69
2	A	801	PHE	CB-CA-C	-2.23	107.28	111.47

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	805	GOL	1	0
3	A	802	TYR	2	0
3	B	802	TYR	1	0
4	A	806	GOL	2	0
4	B	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%)	0.61	40 (5%)	23 26	14, 24, 43, 88	0
1	B	697/720 (96%)	1.41	175 (25%)	0 0	19, 42, 66, 111	0
All	All	1394/1440 (96%)	1.01	215 (15%)	2 2	14, 32, 62, 111	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	523	ALA	9.3
1	B	381	LEU	8.5
1	B	534	LEU	8.3
1	B	620	LEU	7.8
1	B	386	SER	6.8
1	B	144	ASN	6.5
1	A	381	LEU	6.4
1	B	550	THR	6.4
1	B	372	ALA	6.4
1	B	406	ALA	6.3
1	B	376	GLN	6.3
1	B	355	ALA	6.3
1	B	241	ALA	6.3
1	B	135	ALA	6.2
1	B	508	TRP	6.2
1	B	479	LEU	5.9
1	B	94	SER	5.9
1	B	145	ASP	5.8
1	B	432	LEU	5.8
1	B	95	THR	5.5
1	B	618	LYS	5.5
1	B	515	ALA	5.5
1	B	414	ILE	5.4
1	B	516	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	417	SER	5.3
1	B	139	ILE	5.1
1	A	484	ALA	5.0
1	B	68	CYS	4.9
1	B	147	LEU	4.9
1	B	546	GLY	4.9
1	B	543	ILE	4.6
1	B	611	GLU	4.5
1	B	422	GLU	4.5
1	B	168	ALA	4.4
1	B	535	LEU	4.4
1	A	383	THR	4.3
1	B	526	TYR	4.3
1	B	128	ILE	4.2
1	B	383	THR	4.0
1	B	548	SER	4.0
1	B	30	GLN	4.0
1	B	527	ALA	4.0
1	B	229	TYR	3.9
1	B	410	TYR	3.9
1	B	416	ARG	3.8
1	B	360	LEU	3.8
1	B	439	LEU	3.8
1	B	366	ALA	3.8
1	B	712	LEU	3.8
1	B	612	ASP	3.7
1	B	97	GLN	3.7
1	B	367	GLY	3.7
1	A	462	TYR	3.7
1	B	233	ASP	3.5
1	A	79	VAL	3.5
1	B	524	ILE	3.5
1	B	245	PRO	3.5
1	B	364	GLY	3.5
1	B	511	ALA	3.5
1	B	561	ASP	3.5
1	A	365	ALA	3.4
1	B	554	LEU	3.4
1	B	279	LEU	3.4
1	B	378	LEU	3.4
1	B	51	LEU	3.4
1	B	142	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	313	ALA	3.3
1	B	356	VAL	3.3
1	B	358	ALA	3.3
1	B	715	GLU	3.3
1	B	669	LEU	3.3
1	B	626	ALA	3.3
1	B	539	GLU	3.3
1	B	249	LYS	3.2
1	A	35	ILE	3.2
1	A	68	CYS	3.2
1	B	242	ASP	3.2
1	B	39	LEU	3.1
1	B	385	LYS	3.1
1	A	273	ARG	3.1
1	B	622	ASP	3.1
1	B	449	LYS	3.1
1	B	504	THR	3.1
1	B	154	ASP	3.1
1	B	40	GLN	3.1
1	B	359	TRP	3.1
1	B	239	PHE	3.1
1	B	103	ASP	3.0
1	B	520	ASN	3.0
1	B	63	VAL	3.0
1	A	364	GLY	3.0
1	B	363	GLN	3.0
1	B	61	ALA	3.0
1	B	471	ASP	3.0
1	B	653	GLY	2.9
1	B	707	ALA	2.9
1	A	673	GLY	2.9
1	B	231	GLY	2.9
1	A	386	SER	2.9
1	A	89	ALA	2.9
1	A	363	GLN	2.9
1	A	64	ALA	2.9
1	B	126	ASP	2.9
1	B	129	THR	2.9
1	B	172	CYS	2.9
1	B	533	ALA	2.9
1	A	384	SER	2.8
1	B	556	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	35	ILE	2.8
1	B	365	ALA	2.8
1	A	63	VAL	2.8
1	B	435	ILE	2.8
1	B	234	GLY	2.7
1	B	375	ALA	2.7
1	B	604	VAL	2.7
1	B	509	PHE	2.7
1	B	384	SER	2.7
1	B	537	GLN	2.7
1	B	518	ALA	2.7
1	B	463	VAL	2.7
1	B	235	LYS	2.7
1	B	280	ALA	2.7
1	B	402	ALA	2.6
1	B	419	PRO	2.6
1	B	718	LEU	2.6
1	A	660	LEU	2.6
1	B	371	LEU	2.6
1	B	517	GLU	2.6
1	B	582	PHE	2.6
1	B	69	THR	2.6
1	B	638	GLY	2.6
1	B	49	GLU	2.6
1	A	200	PRO	2.6
1	B	109	THR	2.6
1	B	642	VAL	2.5
1	B	706	VAL	2.5
1	B	162	ALA	2.5
1	B	651	THR	2.5
1	B	492	ASN	2.5
1	B	625	LYS	2.5
1	B	710	PRO	2.5
1	B	514	ALA	2.5
1	B	576	LEU	2.5
1	B	273	ARG	2.5
1	B	713	LEU	2.4
1	B	541	LYS	2.4
1	B	559	VAL	2.4
1	A	377	LEU	2.4
1	B	148	ALA	2.4
1	B	380	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	350	GLN	2.4
1	B	362	LYS	2.3
1	B	427	TYR	2.3
1	B	693	ALA	2.3
1	B	170	PHE	2.3
1	B	85	CYS	2.3
1	B	232	LYS	2.3
1	B	87	TYR	2.3
1	B	250	HIS	2.3
1	A	653	GLY	2.3
1	B	114	LEU	2.3
1	B	475	LEU	2.3
1	A	224	SER	2.3
1	A	80	VAL	2.3
1	B	370	ALA	2.3
1	A	367	GLY	2.3
1	A	62	VAL	2.3
1	B	719	ALA	2.3
1	B	568	GLU	2.3
1	A	644	PHE	2.2
1	B	540	GLN	2.2
1	B	658	PRO	2.2
1	B	401	SER	2.2
1	B	692	ILE	2.2
1	A	718	LEU	2.2
1	B	345	ALA	2.2
1	B	265	VAL	2.2
1	A	508	TRP	2.2
1	B	655	SER	2.2
1	A	321	ALA	2.2
1	B	314	ASP	2.2
1	B	270	TYR	2.2
1	B	346	ALA	2.2
1	B	717	ASN	2.2
1	B	522	PRO	2.2
1	B	226	TYR	2.2
1	A	611	GLU	2.2
1	B	443	ASP	2.2
1	A	382	ASP	2.1
1	B	686	PRO	2.1
1	B	127	GLN	2.1
1	B	701	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	530	VAL	2.1
1	A	172	CYS	2.1
1	A	355	ALA	2.1
1	A	374	HIS	2.1
1	B	159	ALA	2.1
1	B	351	ALA	2.1
1	B	560	ALA	2.1
1	B	357	LEU	2.1
1	B	248	PRO	2.1
1	A	550	THR	2.1
1	B	151	ARG	2.1
1	A	366	ALA	2.1
1	A	78	LEU	2.1
1	A	666	LEU	2.1
1	B	67	GLY	2.1
1	B	413	SER	2.0
1	B	28	VAL	2.0
1	B	418	LYS	2.0
1	A	669	LEU	2.0
1	B	377	LEU	2.0
1	A	379	LYS	2.0
1	B	56	GLY	2.0
1	B	545	GLU	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	806	6/6	0.83	0.23	29,37,41,43	0
3	TYR	B	802	13/13	0.84	0.22	23,25,30,31	0
4	GOL	A	805	6/6	0.85	0.14	26,34,37,38	0
4	GOL	B	803	6/6	0.85	0.21	40,42,45,47	0
4	GOL	A	804	6/6	0.86	0.20	30,37,40,41	0
4	GOL	A	803	6/6	0.88	0.23	36,44,46,48	0
2	PHE	B	801	11/12	0.90	0.17	23,27,30,31	0
3	TYR	A	802	13/13	0.92	0.18	17,19,25,25	0
2	PHE	A	801	11/12	0.93	0.16	19,20,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.