



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:12 PM UTC

PDB ID : 7DKD / pdb\_00007dkd  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

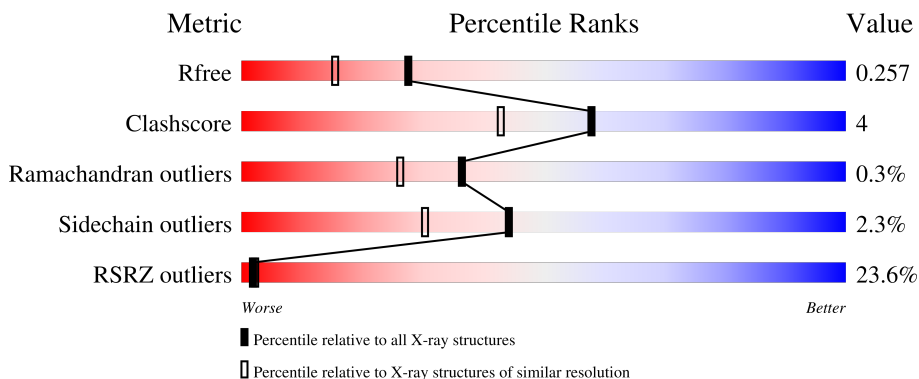
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	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  $\geq 3$ , 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	
1	B	720	

## 2 Entry composition [i](#)

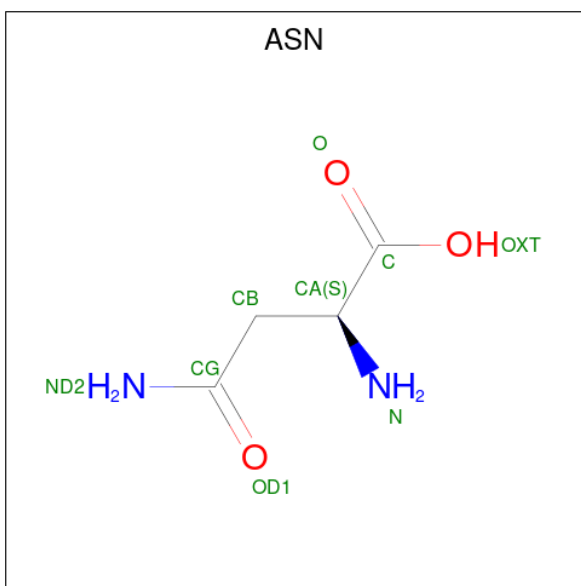
There are 5 unique types of molecules in this entry. The entry contains 11889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

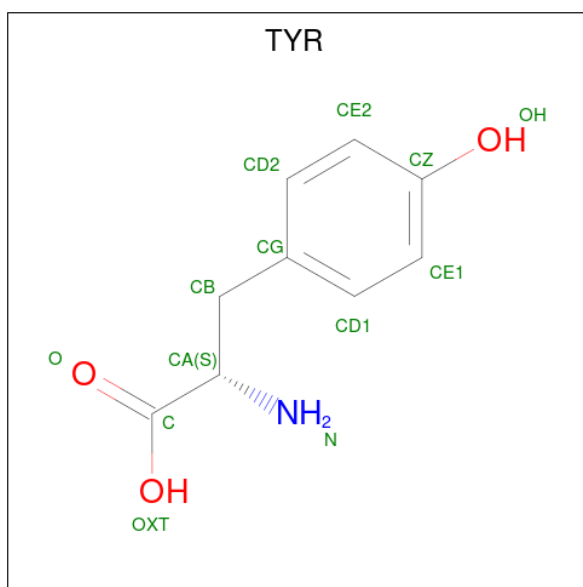
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	697	Total 5329	C 3375	N 927	O 1008	S 19	0	0	0
1	B	697	Total 5338	C 3380	N 928	O 1011	S 19	0	1	0

- Molecule 2 is ASPARAGINE (CCD ID: ASN) (formula:  $C_4H_8N_2O_3$ ).



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

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



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

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



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

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

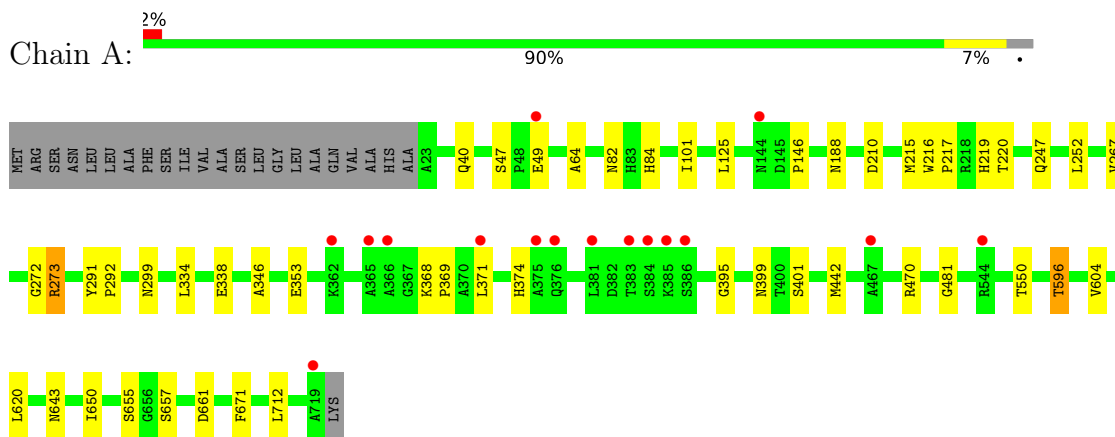
- Molecule 5 is water.

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

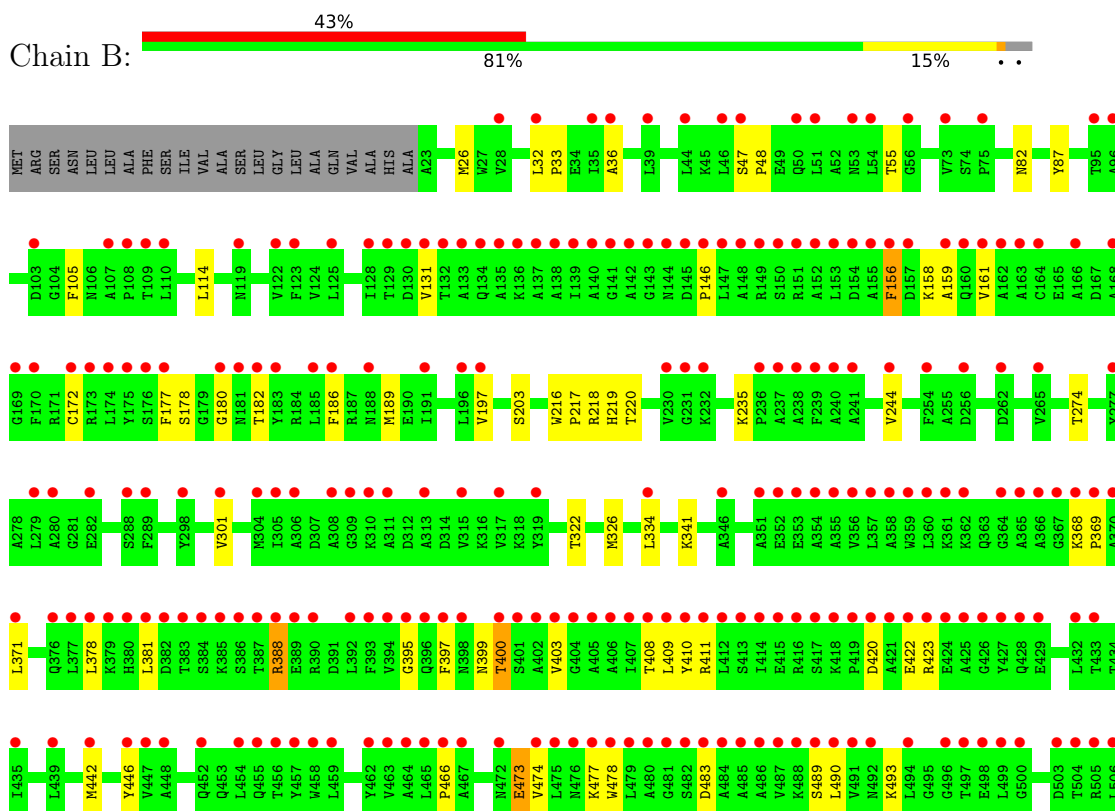
### 3 Residue-property plots [i](#)

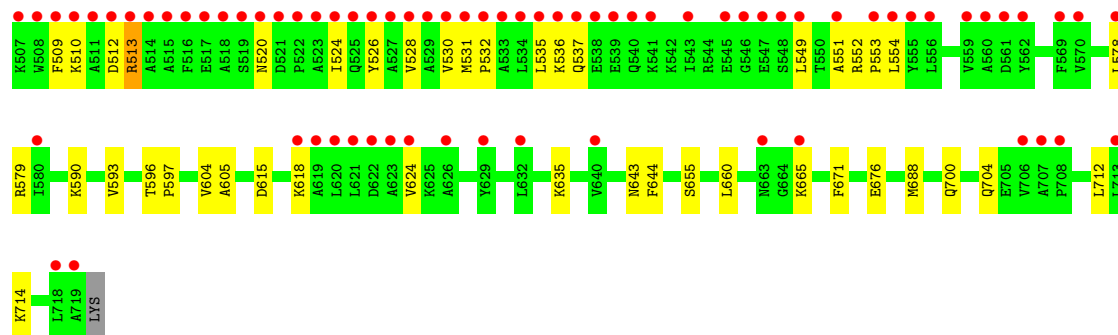
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 40.00 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.92) 99.8 (40.00-1.92)	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)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.202 , 0.248 0.209 , 0.257	Depositor DCC
$R_{free}$ test set	6099 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtrriage
Anisotropy	0.344	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage'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 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	1.08	2/5442 (0.0%)	1.35	8/7375 (0.1%)
1	B	1.07	0/5451	1.49	7/7387 (0.1%)
All	All	1.08	2/10893 (0.0%)	1.42	15/14762 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	LEU	C-O	6.27	1.31	1.23
1	A	650	ILE	C-O	5.54	1.30	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLN	CB-CA-C	5.98	116.87	110.65
1	A	596	THR	CB-CA-C	5.96	117.44	108.86
1	A	661	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	550	THR	CB-CA-C	5.67	118.92	109.56
1	B	466	PRO	CA-C-N	5.60	128.10	120.54
1	B	466	PRO	C-N-CA	5.60	128.10	120.54
1	A	101	ILE	N-CA-C	-5.55	105.09	110.42
1	B	483	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	483	ASP	CA-C-N	5.33	128.16	120.38
1	B	483	ASP	C-N-CA	5.33	128.16	120.38
1	B	87	TYR	CA-C-N	5.26	125.82	119.98
1	B	87	TYR	C-N-CA	5.26	125.82	119.98
1	A	346	ALA	CA-C-N	5.24	125.77	120.00
1	A	346	ALA	C-N-CA	5.24	125.77	120.00
1	A	481	GLY	CA-C-O	-5.01	116.85	121.96

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	31	0
1	B	5338	0	5276	62	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	95	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 (95) 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
1:B:531:MET:HE3	1:B:535:LEU:HG	1.75	0.66
4:A:804:GOL:H31	5:A:1495:HOH:O	1.98	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:655:SER:OG	3:A:802:TYR:C	2.49	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:442:MET:HE3	1:B:446:TYR:CD2	2.42	0.55
1:B:655:SER:OG	3:B:802:TYR:C	2.51	0.54
1:B:512:ASP:O	1:B:513:ARG:HB2	2.07	0.53
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:B:605:ALA:HB2	1:B:624:VAL:HG11	1.92	0.50
1:B:156:PHE:C	1:B:156:PHE:CD1	2.88	0.50
1:B:301:VAL:HG11	1:B:326:MET:HE1	1.93	0.50
1:B:474:VAL:O	1:B:477:LYS:HB3	2.12	0.50
1:B:301:VAL:CG1	1:B:326:MET:HE1	2.41	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: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:A:401:SER:HB3	1:A:442:MET:HE3	1.94	0.48
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:A:620:LEU:HD23	1:A:620:LEU:C	2.40	0.46
1:B:158:LYS:NZ	1:B:423:ARG:O	2.48	0.46
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:B:714:LYS:NZ	5:B:908:HOH:O	2.47	0.46
1:A:267:VAL:HG13	1:A:657:SER:HB3	1.98	0.46
1:B:420:ASP:C	1:B:422:GLU:H	2.24	0.46
1:B:531:MET:N	1:B:532:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:26:MET:HE1	1:B:274:THR:HG21	1.99	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: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
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:411:ARG:HD3	1:B:531:MET:HE1	2.03	0.41
1:B:197:VAL:CG1	1:B:712:LEU:HD21	2.48	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:216:TRP:HA	1:B:217:PRO:C	2.47	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 [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%)	676 (97%)	19 (3%)	0	100	100
1	B	696/720 (97%)	643 (92%)	49 (7%)	4 (1%)	21	10
All	All	1391/1440 (97%)	1319 (95%)	68 (5%)	4 (0%)	36	26

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 [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%)	70	67
1	B	541/557 (97%)	521 (96%)	20 (4%)	30	15
All	All	1081/1114 (97%)	1056 (98%)	25 (2%)	44	30

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	49	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	215	MET
1	A	273	ARG
1	A	712	LEU
1	B	55	THR
1	B	156	PHE
1	B	161	VAL
1	B	235	LYS
1	B	322	THR
1	B	371	LEU
1	B	378	LEU
1	B	381	LEU
1	B	388	ARG
1	B	400	THR
1	B	408	THR
1	B	473	GLU
1	B	489	SER
1	B	493	LYS
1	B	520	ASN
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 (30) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	40	GLN
1	A	82	ASN
1	A	144	ASN
1	A	188	ASN
1	A	213	ASN
1	A	247	GLN
1	A	275	ASN
1	A	299	ASN
1	A	327	ASN
1	A	328	ASN
1	A	336	GLN
1	A	350	GLN
1	A	374	HIS
1	A	584	ASN
1	A	643	ASN

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Mol	Chain	Res	Type
1	A	654	ASN
1	A	681	ASN
1	B	50	GLN
1	B	82	ASN
1	B	160	GLN
1	B	213	ASN
1	B	275	ASN
1	B	328	ASN
1	B	336	GLN
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 oligosaccharides 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
2	ASN	B	801	3	6,7,8	0.90	0	4,8,10	0.41	0
3	TYR	B	802	2	12,13,13	0.56	0	13,17,17	0.65	1 (7%)
3	TYR	A	802	2	12,13,13	0.79	1 (8%)	13,17,17	0.78	1 (7%)
4	GOL	A	805	-	5,5,5	0.15	0	5,5,5	0.32	0
2	ASN	A	801	3	6,7,8	0.91	0	4,8,10	0.63	0
4	GOL	A	804	-	5,5,5	0.25	0	5,5,5	0.43	0
4	GOL	A	803	-	5,5,5	0.24	0	5,5,5	0.61	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	ASN	B	801	3	-	0/5/6/8	-
3	TYR	B	802	2	-	6/8/8/8	0/1/1/1
3	TYR	A	802	2	-	5/8/8/8	0/1/1/1
4	GOL	A	805	-	-	4/4/4/4	-
2	ASN	A	801	3	-	0/5/6/8	-
4	GOL	A	804	-	-	1/4/4/4	-
4	GOL	A	803	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	TYR	OXT-C	-2.59	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	TYR	OXT-C-O	-2.09	119.33	124.08
3	B	802	TYR	OXT-C-O	-2.01	119.52	124.08

There are no chirality outliers.

All (18) 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

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

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	TYR	1	0
3	A	802	TYR	1	0
4	A	804	GOL	2	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%)	-0.10	16 (2%) 61 67	6, 15, 35, 73	0
1	B	697/720 (96%)	1.97	313 (44%) 0 0	10, 45, 78, 105	1 (0%)
All	All	1394/1440 (96%)	0.93	329 (23%) 2 2	6, 26, 71, 105	1 (0%)

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	535	LEU	7.0
1	B	511	ALA	6.7
1	B	142	ALA	6.4
1	B	719	ALA	6.4
1	B	516	PHE	6.3
1	B	524	ILE	6.3
1	B	414	ILE	6.2
1	B	479	LEU	6.2
1	B	534	LEU	6.1
1	B	410	TYR	6.1
1	B	139	ILE	6.1
1	B	499	LEU	6.0
1	B	515	ALA	5.9
1	B	523	ALA	5.9
1	B	526	TYR	5.7
1	B	135	ALA	5.6
1	B	491	VAL	5.5
1	B	360	LEU	5.4
1	B	475	LEU	5.4
1	B	406	ALA	5.3
1	B	412	LEU	5.2
1	B	159	ALA	5.1
1	B	423	ARG	5.1
1	B	421	ALA	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	393	PHE	5.1
1	B	478	TRP	5.0
1	B	529	ALA	5.0
1	B	356	VAL	5.0
1	B	530	VAL	4.9
1	B	484	ALA	4.9
1	B	533	ALA	4.9
1	B	514	ALA	4.9
1	B	381	LEU	4.8
1	B	508	TRP	4.8
1	B	425	ALA	4.8
1	B	522	PRO	4.8
1	B	378	LEU	4.7
1	B	146	PRO	4.7
1	B	153	LEU	4.7
1	B	543	ILE	4.6
1	B	487	VAL	4.5
1	B	140	ALA	4.5
1	B	155	ALA	4.4
1	A	719	ALA	4.4
1	B	409	LEU	4.3
1	B	494	LEU	4.3
1	B	313	ALA	4.3
1	B	481	GLY	4.3
1	B	432	LEU	4.2
1	B	549	LEU	4.2
1	B	397	PHE	4.2
1	B	485	ALA	4.2
1	B	385	LYS	4.2
1	B	162	ALA	4.0
1	B	163	ALA	4.0
1	B	459	LEU	4.0
1	B	532	PRO	4.0
1	B	131	VAL	4.0
1	B	133	ALA	4.0
1	B	315	VAL	4.0
1	B	355	ALA	4.0
1	B	463	VAL	4.0
1	B	518	ALA	4.0
1	A	384	SER	4.0
1	B	490	LEU	4.0
1	B	138	ALA	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	402	ALA	4.0
1	B	417	SER	4.0
1	B	383	THR	3.9
1	B	555	TYR	3.9
1	B	474	VAL	3.9
1	B	46	LEU	3.9
1	B	311	ALA	3.9
1	B	528	VAL	3.9
1	B	392	LEU	3.8
1	B	554	LEU	3.8
1	B	148	ALA	3.8
1	B	359	TRP	3.8
1	B	405	ALA	3.8
1	B	486	ALA	3.8
1	B	132	THR	3.7
1	B	454	LEU	3.7
1	B	176	SER	3.7
1	B	169	GLY	3.7
1	B	183	TYR	3.7
1	B	143	GLY	3.7
1	B	525	GLN	3.7
1	B	458	TRP	3.7
1	B	305	ILE	3.6
1	B	156	PHE	3.6
1	B	386	SER	3.6
1	B	137	ALA	3.6
1	B	465	LEU	3.6
1	B	164	CYS	3.6
1	B	408	THR	3.6
1	B	506	LEU	3.6
1	B	400	THR	3.5
1	B	407	ILE	3.5
1	B	620	LEU	3.5
1	B	446	TYR	3.5
1	B	128	ILE	3.5
1	B	185	LEU	3.5
1	B	556	LEU	3.5
1	B	545	GLU	3.4
1	B	371	LEU	3.4
1	B	394	VAL	3.4
1	B	154	ASP	3.4
1	B	241	ALA	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	540	GLN	3.4
1	B	560	ALA	3.4
1	B	366	ALA	3.4
1	B	351	ALA	3.3
1	B	546	GLY	3.3
1	B	280	ALA	3.3
1	B	477	LYS	3.3
1	B	401	SER	3.3
1	B	527	ALA	3.2
1	B	626	ALA	3.2
1	B	718	LEU	3.2
1	B	180	GLY	3.2
1	B	435	ILE	3.2
1	B	161	VAL	3.2
1	B	424	GLU	3.2
1	B	141	GLY	3.2
1	B	231	GLY	3.2
1	B	482	SER	3.2
1	B	427	TYR	3.2
1	B	147	LEU	3.2
1	A	386	SER	3.2
1	B	170	PHE	3.2
1	B	507	LYS	3.1
1	B	54	LEU	3.1
1	B	624	VAL	3.1
1	B	177	PHE	3.1
1	B	354	ALA	3.1
1	B	462	TYR	3.1
1	B	145	ASP	3.1
1	B	186	PHE	3.1
1	B	618	LYS	3.1
1	B	413	SER	3.1
1	B	416	ARG	3.1
1	B	489	SER	3.1
1	B	36	ALA	3.1
1	B	35	ILE	3.0
1	B	244	VAL	3.0
1	B	500	GLY	3.0
1	B	707	ALA	3.0
1	B	191	ILE	3.0
1	B	384	SER	3.0
1	B	364	GLY	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	365	ALA	3.0
1	B	32	LEU	3.0
1	B	149	ARG	3.0
1	B	152	ALA	3.0
1	A	381	LEU	2.9
1	B	562	TYR	2.9
1	B	395	GLY	2.9
1	B	456	THR	2.9
1	B	517	GLU	2.9
1	B	279	LEU	2.9
1	B	377	LEU	2.9
1	B	420	ASP	2.9
1	B	239	PHE	2.9
1	B	237	ALA	2.9
1	B	380	HIS	2.9
1	B	510	LYS	2.9
1	B	108	PRO	2.9
1	B	419	PRO	2.9
1	B	623	ALA	2.9
1	B	483	ASP	2.9
1	B	357	LEU	2.9
1	B	426	GLY	2.9
1	B	520	ASN	2.8
1	B	168	ALA	2.8
1	B	346	ALA	2.8
1	B	504	THR	2.8
1	B	466	PRO	2.8
1	B	157	ASP	2.8
1	B	308	ALA	2.8
1	B	398	ASN	2.8
1	B	498	GLU	2.8
1	B	538	GLU	2.8
1	B	448	ALA	2.8
1	A	383	THR	2.8
1	B	238	ALA	2.7
1	B	361	LYS	2.7
1	B	569	PHE	2.7
1	B	150	SER	2.7
1	B	144	ASN	2.7
1	B	476	ASN	2.7
1	B	492	ASN	2.7
1	B	447	VAL	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	570	VAL	2.7
1	A	467	ALA	2.7
1	B	166	ALA	2.7
1	B	387	THR	2.7
1	B	418	LYS	2.7
1	A	365	ALA	2.6
1	B	175	TYR	2.6
1	B	289	PHE	2.6
1	B	39	LEU	2.6
1	B	230	VAL	2.6
1	B	496	GLY	2.6
1	B	306	ALA	2.6
1	B	382	ASP	2.6
1	B	513	ARG	2.6
1	B	428	GLN	2.6
1	B	539	GLU	2.6
1	B	136	LYS	2.6
1	B	334	LEU	2.6
1	B	411	ARG	2.6
1	B	358	ALA	2.6
1	B	232	LYS	2.6
1	B	488	LYS	2.6
1	B	548	SER	2.6
1	B	110	LEU	2.6
1	B	379	LYS	2.6
1	B	122	VAL	2.6
1	B	376	GLN	2.5
1	B	429	GLU	2.5
1	B	309	GLY	2.5
1	B	301	VAL	2.5
1	B	403	VAL	2.5
1	B	531	MET	2.5
1	B	367	GLY	2.5
1	B	288	SER	2.5
1	B	467	ALA	2.5
1	B	559	VAL	2.5
1	B	521	ASP	2.5
1	A	385	LYS	2.5
1	B	665	LYS	2.5
1	B	172	CYS	2.5
1	B	621	LEU	2.5
1	B	282	GLU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	452	GLN	2.5
1	B	182	THR	2.5
1	B	553	PRO	2.5
1	B	509	PHE	2.4
1	B	129	THR	2.4
1	B	561	ASP	2.4
1	B	125	LEU	2.4
1	B	629	TYR	2.4
1	B	160	GLN	2.4
1	B	442	MET	2.4
1	B	457	TYR	2.4
1	B	580	ILE	2.4
1	B	472	ASN	2.4
1	B	519	SER	2.4
1	B	256	ASP	2.3
1	B	51	LEU	2.3
1	B	439	LEU	2.3
1	B	713	LEU	2.3
1	B	109	THR	2.3
1	B	497	THR	2.3
1	B	537	GLN	2.3
1	B	536	LYS	2.3
1	B	317	VAL	2.3
1	B	640	VAL	2.3
1	B	706	VAL	2.3
1	B	352	GLU	2.3
1	B	134	GLN	2.3
1	B	304	MET	2.3
1	B	197	VAL	2.3
1	B	512	ASP	2.3
1	B	551	ALA	2.3
1	B	53	ASN	2.3
1	B	181	ASN	2.3
1	A	375	ALA	2.2
1	B	480	ALA	2.2
1	B	619	ALA	2.2
1	B	503	ASP	2.2
1	B	362	LYS	2.2
1	B	389	GLU	2.2
1	A	366	ALA	2.2
1	B	123	PHE	2.2
1	B	310	LYS	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	368	LYS	2.2
1	B	95	THR	2.2
1	A	371	LEU	2.2
1	B	174	LEU	2.2
1	B	369	PRO	2.2
1	B	298	TYR	2.2
1	B	319	TYR	2.2
1	B	663	ASN	2.2
1	A	49	GLU	2.2
1	B	103	ASP	2.2
1	B	130	ASP	2.2
1	B	632	LEU	2.2
1	B	107	ALA	2.2
1	B	240	ALA	2.2
1	B	464	ALA	2.2
1	B	547	GLU	2.1
1	B	622	ASP	2.1
1	B	404	GLY	2.1
1	B	415	GLU	2.1
1	B	96	ALA	2.1
1	B	119	ASN	2.1
1	B	254	PHE	2.1
1	B	47	SER	2.1
1	B	505	ARG	2.1
1	A	362	LYS	2.1
1	B	541	LYS	2.1
1	B	277	TYR	2.1
1	B	433	THR	2.1
1	A	144	ASN	2.1
1	B	28	VAL	2.1
1	B	73	VAL	2.1
1	A	376	GLN	2.1
1	B	50	GLN	2.1
1	B	396	GLN	2.1
1	B	44	LEU	2.1
1	B	196	LEU	2.1
1	B	578	LEU	2.1
1	B	262	ASP	2.1
1	B	390	ARG	2.1
1	B	353	GLU	2.0
1	B	56	GLY	2.0
1	B	455	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	236	PRO	2.0
1	B	265	VAL	2.0
1	B	708	PRO	2.0
1	A	544	ARG	2.0
1	B	151	ARG	2.0
1	B	370	ALA	2.0
1	B	422	GLU	2.0
1	B	188	ASN	2.0
1	B	75	PRO	2.0
1	B	173	ARG	2.0
1	B	388	ARG	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, 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(Å <sup>2</sup> )	Q<0.9
4	GOL	A	805	6/6	0.78	0.19	32,38,41,42	0
3	TYR	B	802	13/13	0.87	0.12	21,25,28,34	0
4	GOL	A	804	6/6	0.88	0.14	18,25,27,28	0
4	GOL	A	803	6/6	0.88	0.11	23,28,29,30	0
2	ASN	A	801	8/9	0.93	0.08	11,13,14,14	0
2	ASN	B	801	8/9	0.93	0.08	23,24,28,31	0
3	TYR	A	802	13/13	0.94	0.08	13,16,18,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.