



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:02 PM BST

PDB ID : 5ZRD  
Title : Tyrosinase from Burkholderia thailandensis (BtTYR) at low pH condition  
Authors : Lee, S.; Son, H.-F.; Kim, K.-J.  
Deposited on : 2018-04-24  
Resolution : 2.30 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 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 : 2.13.1  
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) : 2.13.1

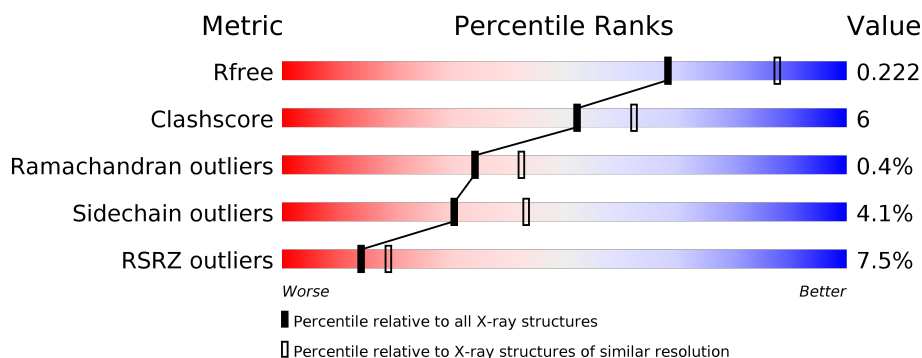
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	549	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	549	<div> <div>10%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </div>
1	C	549	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	D	549	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	602	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17209 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4163	2646	717	787	13			
1	B	531	Total	C	N	O	S	0	0	0
			4140	2631	713	783	13			
1	C	529	Total	C	N	O	S	0	0	0
			4123	2621	710	779	13			
1	D	528	Total	C	N	O	S	0	0	0
			4118	2618	709	778	13			

There are 60 discrepancies between the modelled and reference sequences:

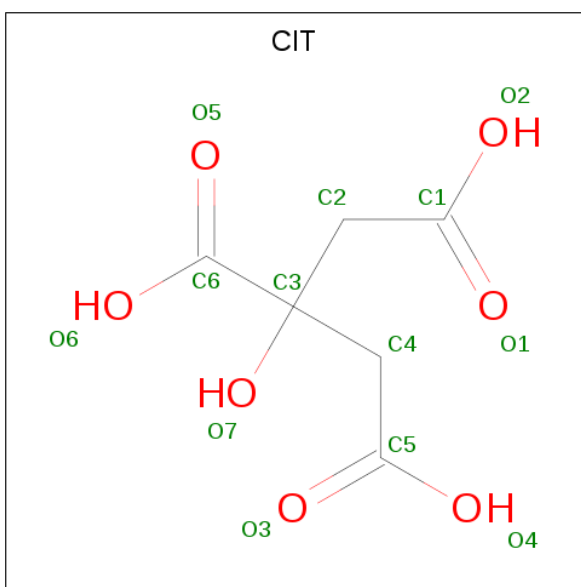
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q2T7K1
A	1	GLY	-	expression tag	UNP Q2T7K1
A	536	LYS	-	expression tag	UNP Q2T7K1
A	537	LEU	-	expression tag	UNP Q2T7K1
A	538	ALA	-	expression tag	UNP Q2T7K1
A	539	ALA	-	expression tag	UNP Q2T7K1
A	540	ALA	-	expression tag	UNP Q2T7K1
A	541	LEU	-	expression tag	UNP Q2T7K1
A	542	GLU	-	expression tag	UNP Q2T7K1
A	543	HIS	-	expression tag	UNP Q2T7K1
A	544	HIS	-	expression tag	UNP Q2T7K1
A	545	HIS	-	expression tag	UNP Q2T7K1
A	546	HIS	-	expression tag	UNP Q2T7K1
A	547	HIS	-	expression tag	UNP Q2T7K1
A	548	HIS	-	expression tag	UNP Q2T7K1
B	0	MET	-	expression tag	UNP Q2T7K1
B	1	GLY	-	expression tag	UNP Q2T7K1
B	536	LYS	-	expression tag	UNP Q2T7K1
B	537	LEU	-	expression tag	UNP Q2T7K1
B	538	ALA	-	expression tag	UNP Q2T7K1
B	539	ALA	-	expression tag	UNP Q2T7K1

*Continued on next page...*

*Continued from previous page...*

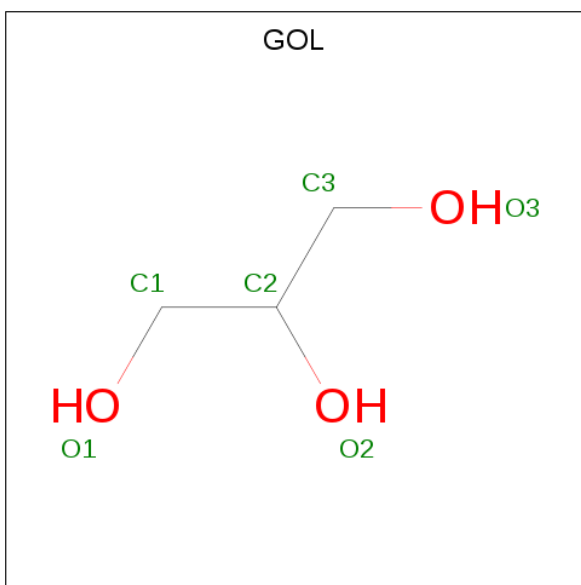
Chain	Residue	Modelled	Actual	Comment	Reference
B	540	ALA	-	expression tag	UNP Q2T7K1
B	541	LEU	-	expression tag	UNP Q2T7K1
B	542	GLU	-	expression tag	UNP Q2T7K1
B	543	HIS	-	expression tag	UNP Q2T7K1
B	544	HIS	-	expression tag	UNP Q2T7K1
B	545	HIS	-	expression tag	UNP Q2T7K1
B	546	HIS	-	expression tag	UNP Q2T7K1
B	547	HIS	-	expression tag	UNP Q2T7K1
B	548	HIS	-	expression tag	UNP Q2T7K1
C	0	MET	-	expression tag	UNP Q2T7K1
C	1	GLY	-	expression tag	UNP Q2T7K1
C	536	LYS	-	expression tag	UNP Q2T7K1
C	537	LEU	-	expression tag	UNP Q2T7K1
C	538	ALA	-	expression tag	UNP Q2T7K1
C	539	ALA	-	expression tag	UNP Q2T7K1
C	540	ALA	-	expression tag	UNP Q2T7K1
C	541	LEU	-	expression tag	UNP Q2T7K1
C	542	GLU	-	expression tag	UNP Q2T7K1
C	543	HIS	-	expression tag	UNP Q2T7K1
C	544	HIS	-	expression tag	UNP Q2T7K1
C	545	HIS	-	expression tag	UNP Q2T7K1
C	546	HIS	-	expression tag	UNP Q2T7K1
C	547	HIS	-	expression tag	UNP Q2T7K1
C	548	HIS	-	expression tag	UNP Q2T7K1
D	0	MET	-	expression tag	UNP Q2T7K1
D	1	GLY	-	expression tag	UNP Q2T7K1
D	536	LYS	-	expression tag	UNP Q2T7K1
D	537	LEU	-	expression tag	UNP Q2T7K1
D	538	ALA	-	expression tag	UNP Q2T7K1
D	539	ALA	-	expression tag	UNP Q2T7K1
D	540	ALA	-	expression tag	UNP Q2T7K1
D	541	LEU	-	expression tag	UNP Q2T7K1
D	542	GLU	-	expression tag	UNP Q2T7K1
D	543	HIS	-	expression tag	UNP Q2T7K1
D	544	HIS	-	expression tag	UNP Q2T7K1
D	545	HIS	-	expression tag	UNP Q2T7K1
D	546	HIS	-	expression tag	UNP Q2T7K1
D	547	HIS	-	expression tag	UNP Q2T7K1
D	548	HIS	-	expression tag	UNP Q2T7K1

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Cu 2 2	0	0
4	A	2	Total Cu 2 2	0	0
4	D	2	Total Cu 2 2	0	0
4	C	2	Total Cu 2 2	0	0

- Molecule 5 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	O 1	0	0
5	A	1	Total 1	O 1	0	0
5	D	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0

- Molecule 6 is water.

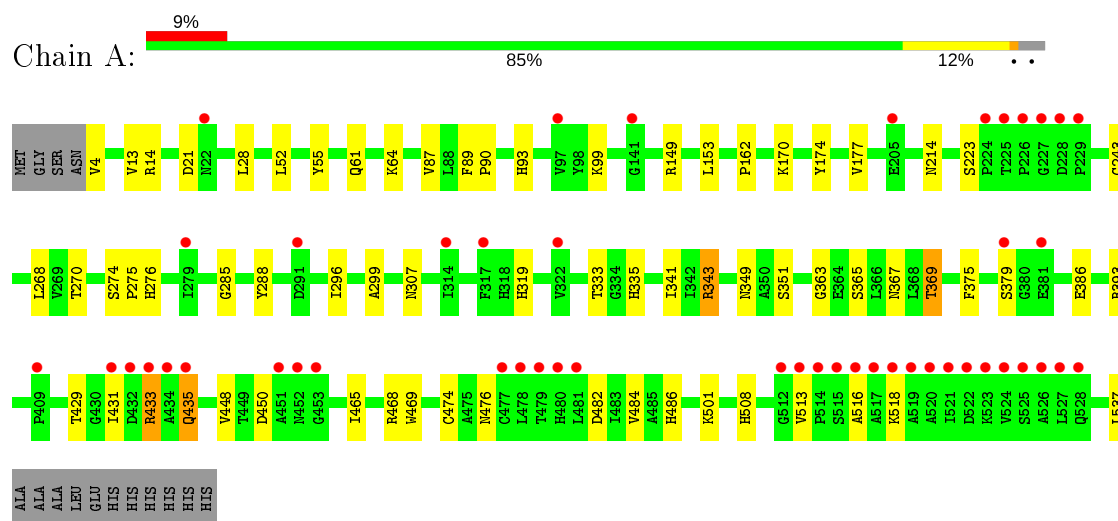
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	160	Total 160	O 160	0	0
6	B	139	Total 139	O 139	0	0
6	C	102	Total 102	O 102	0	0
6	D	116	Total 116	O 116	0	0



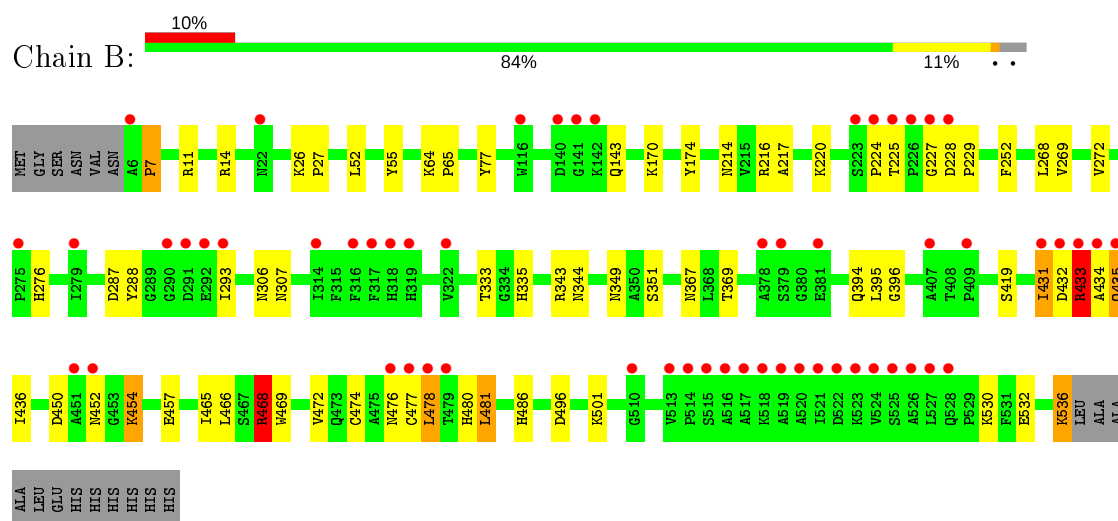
### 3 Residue-property plots [i](#)

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.

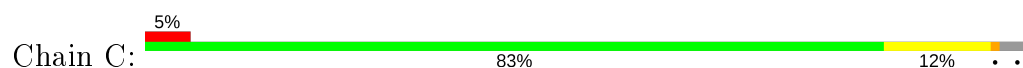
#### • Molecule 1: Tyrosinase

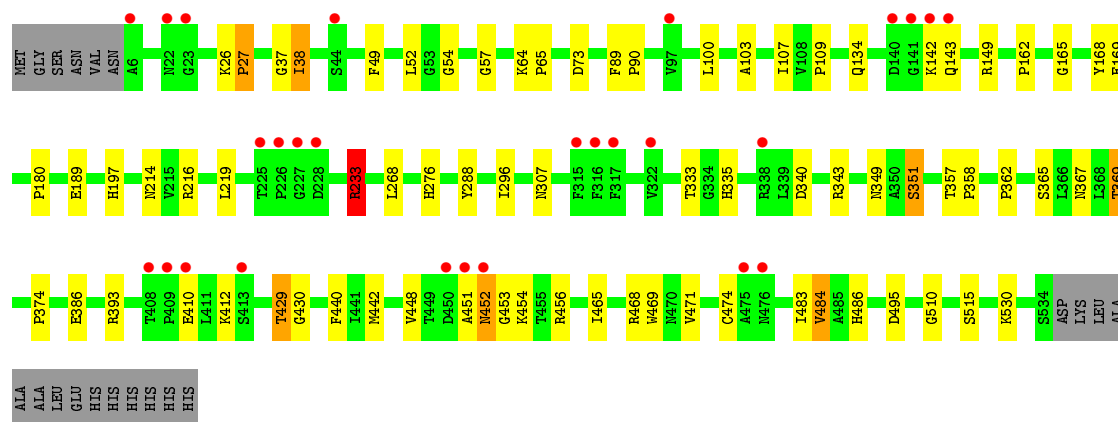


#### • Molecule 1: Tyrosinase

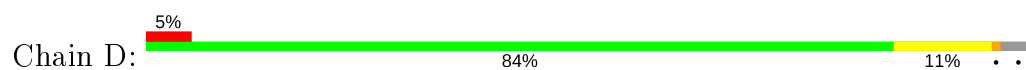


#### • Molecule 1: Tyrosinase





• Molecule 1: Tyrosinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.91Å 142.91Å 256.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.88 – 2.30 28.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.88-2.30) 97.9 (28.86-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.27 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.180 , 0.221 0.187 , 0.222	Depositor DCC
$R_{free}$ test set	6679 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6570e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, O, CU, CIT

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	0.64	0/4282	0.80	1/5834 (0.0%)
1	B	0.63	0/4259	0.81	3/5802 (0.1%)
1	C	0.59	0/4242	0.79	2/5780 (0.0%)
1	D	0.61	0/4237	0.77	0/5772
All	All	0.62	0/17020	0.79	6/23188 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	3
1	D	0	1
All	All	0	10

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	468	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	C	73	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	496	ASP	CB-CG-OD1	5.58	123.33	118.30
1	B	468	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	21	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	468	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	393	ARG	Sidechain
1	B	11	ARG	Sidechain
1	B	216	ARG	Sidechain
1	B	433	ARG	Sidechain
1	B	476	ASN	Peptide
1	C	149	ARG	Sidechain
1	C	216	ARG	Sidechain
1	C	233	ARG	Sidechain
1	D	19	ARG	Sidechain

## 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	4163	0	4043	49	0
1	B	4140	0	4017	46	0
1	C	4123	0	3998	46	0
1	D	4118	0	3994	43	0
2	A	13	0	5	2	0
2	B	13	0	5	1	0
2	C	13	0	5	4	0
2	D	13	0	5	4	0
3	A	24	0	32	11	0
3	B	24	0	32	3	0
3	C	12	0	16	3	0
3	D	24	0	32	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	160	0	0	2	0
6	B	139	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	102	0	0	2	0
6	D	116	0	0	1	0
All	All	17209	0	16184	182	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 6.

All (182) 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:A:468:ARG:HH12	3:A:602:GOL:C3	1.73	1.01
1:A:468:ARG:HH12	3:A:602:GOL:H32	1.26	0.98
1:C:486:HIS:HD2	2:C:601:CIT:O1	1.48	0.96
2:C:601:CIT:O3	2:C:601:CIT:H22	1.61	0.96
1:C:486:HIS:CD2	2:C:601:CIT:O1	2.28	0.85
2:D:601:CIT:O4	2:D:601:CIT:H22	1.77	0.84
1:A:468:ARG:NH1	3:A:602:GOL:H32	1.95	0.81
1:B:349:ASN:HD22	1:B:351:SER:H	1.26	0.81
1:A:468:ARG:HH22	3:A:602:GOL:H31	1.47	0.79
1:D:349:ASN:HD22	1:D:351:SER:H	1.29	0.78
1:C:349:ASN:HD22	1:C:351:SER:H	1.29	0.78
1:A:468:ARG:NH1	3:A:602:GOL:C3	2.47	0.78
1:C:367:ASN:OD1	1:C:369:THR:HB	1.86	0.75
2:C:601:CIT:O3	2:C:601:CIT:C2	2.34	0.75
1:A:349:ASN:HD22	1:A:351:SER:H	1.35	0.73
1:D:486:HIS:HD2	2:D:601:CIT:O2	1.70	0.73
1:C:296:ILE:HD12	1:C:510:GLY:HA3	1.72	0.70
1:A:468:ARG:NH2	3:A:602:GOL:H31	2.06	0.70
1:C:307:ASN:HD21	1:C:469:TRP:H	1.41	0.68
1:B:450:ASP:O	1:B:452:ASN:HA	1.95	0.65
1:C:296:ILE:HD12	1:C:510:GLY:CA	2.27	0.65
1:B:432:ASP:O	1:B:434:ALA:N	2.30	0.64
1:C:349:ASN:ND2	1:C:351:SER:H	1.95	0.64
1:D:214:ASN:HD21	1:D:288:TYR:H	1.45	0.63
1:A:307:ASN:ND2	1:A:469:TRP:H	1.97	0.63
1:B:436:ILE:HG21	1:B:481:LEU:HD23	1.80	0.63
1:A:468:ARG:HH12	3:A:602:GOL:H31	1.61	0.63
1:D:349:ASN:ND2	1:D:351:SER:H	1.95	0.62
1:D:307:ASN:HD21	1:D:469:TRP:H	1.47	0.62
1:B:227:GLY:HA3	1:B:228:ASP:HB2	1.82	0.62
1:C:307:ASN:ND2	1:C:469:TRP:H	1.98	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:PRO:O	1:C:197:HIS:HE1	1.84	0.60
1:A:468:ARG:NH1	3:A:602:GOL:H31	2.15	0.60
1:A:484:VAL:HG11	1:B:344:ASN:ND2	2.17	0.60
1:C:349:ASN:HD22	1:C:351:SER:HB2	1.65	0.60
1:D:307:ASN:ND2	1:D:469:TRP:H	1.99	0.60
1:B:435:GLN:HG3	1:B:478:LEU:HD12	1.85	0.59
1:A:307:ASN:HD21	1:A:469:TRP:H	1.49	0.59
1:B:536:LYS:N	1:B:536:LYS:HD3	2.18	0.59
1:C:189:GLU:OE2	1:C:515:SER:N	2.36	0.59
1:A:61:GLN:NE2	6:A:703:HOH:O	2.36	0.58
1:C:307:ASN:HD21	1:C:469:TRP:N	2.01	0.58
1:C:429:THR:HG22	1:C:530:LYS:HB3	1.86	0.58
1:A:367:ASN:OD1	1:A:369:THR:HB	2.04	0.58
1:D:486:HIS:CD2	2:D:601:CIT:O2	2.54	0.58
1:A:162:PRO:HD2	1:D:472:VAL:HG23	1.87	0.57
1:B:214:ASN:HD21	1:B:287:ASP:HA	1.69	0.57
1:C:38:ILE:HG23	1:C:49:PHE:HB2	1.86	0.57
1:D:174:TYR:HA	3:D:605:GOL:H2	1.87	0.57
1:A:474:CYS:HB2	1:A:476:ASN:OD1	2.04	0.57
1:B:349:ASN:ND2	1:B:351:SER:H	2.01	0.56
2:D:601:CIT:O4	2:D:601:CIT:C2	2.51	0.56
1:C:349:ASN:ND2	1:C:351:SER:HB2	2.20	0.56
1:D:296:ILE:HD12	1:D:510:GLY:HA3	1.87	0.56
1:A:433:ARG:CZ	1:A:435:GLN:HE22	2.19	0.56
1:A:343:ARG:NH1	1:B:532:GLU:OE2	2.39	0.56
1:B:14:ARG:HH21	3:B:602:GOL:C1	2.19	0.55
1:A:333:THR:OG1	1:A:335:HIS:HD2	1.88	0.55
1:B:433:ARG:HD3	1:B:480:HIS:HB3	1.88	0.55
1:A:274:SER:HB3	1:A:275:PRO:CD	2.37	0.55
1:A:153:LEU:HD12	1:A:174:TYR:HB3	1.88	0.54
1:B:214:ASN:ND2	1:B:287:ASP:HA	2.22	0.54
1:D:335:HIS:HE1	6:D:702:HOH:O	1.91	0.53
1:D:64:LYS:N	1:D:65:PRO:CD	2.71	0.53
1:B:26:LYS:N	1:B:27:PRO:HD2	2.24	0.53
1:A:214:ASN:HD21	1:A:288:TYR:H	1.53	0.53
1:A:468:ARG:CZ	3:A:602:GOL:H31	2.37	0.53
1:B:450:ASP:C	1:B:452:ASN:HA	2.28	0.53
1:D:123:THR:HG22	1:D:219:LEU:CD1	2.39	0.53
1:B:306:ASN:HD21	1:B:466:LEU:HD21	1.73	0.52
1:D:214:ASN:ND2	1:D:288:TYR:H	2.06	0.52
1:C:214:ASN:HD21	1:C:288:TYR:H	1.57	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:GLY:HA2	1:D:169:GLU:OE2	2.09	0.52
1:D:307:ASN:HD21	1:D:469:TRP:N	2.07	0.52
1:A:513:VAL:CG2	1:A:516:ALA:HB3	2.39	0.52
1:B:367:ASN:HB2	6:B:819:HOH:O	2.08	0.52
1:B:486:HIS:HD2	2:B:601:CIT:O1	1.93	0.52
1:B:227:GLY:CA	1:B:228:ASP:HB2	2.40	0.51
1:C:165:GLY:HA2	1:C:169:GLU:OE1	2.11	0.51
1:A:93:HIS:CD2	1:A:319:HIS:CE1	2.99	0.51
1:D:386:GLU:HA	1:D:386:GLU:OE2	2.11	0.51
1:D:388:CYS:HB2	1:D:395:LEU:HD11	1.92	0.50
1:B:333:THR:OG1	1:B:335:HIS:HD2	1.94	0.50
1:C:57:GLY:O	6:C:701:HOH:O	2.20	0.50
1:D:268:LEU:HD23	1:D:425:LYS:HE2	1.94	0.50
1:B:307:ASN:ND2	1:B:469:TRP:H	2.10	0.50
1:D:241:VAL:HG12	1:D:415:LEU:HD11	1.94	0.50
1:C:26:LYS:N	1:C:27:PRO:CD	2.76	0.49
1:D:124:LEU:HB3	1:D:229:PRO:HB3	1.93	0.49
1:A:484:VAL:HG11	1:B:344:ASN:HD21	1.75	0.49
1:A:307:ASN:HD21	1:A:469:TRP:N	2.10	0.49
1:C:465:ILE:HD12	1:C:465:ILE:N	2.27	0.48
1:D:170:LYS:HE2	1:D:174:TYR:CE2	2.48	0.48
1:D:336:THR:CG2	1:D:390:ASN:ND2	2.76	0.48
1:A:296:ILE:CD1	1:A:508:HIS:CE1	2.97	0.48
1:D:135:GLU:HA	1:D:149:ARG:HD3	1.95	0.48
1:A:170:LYS:HE3	1:A:174:TYR:CZ	2.48	0.48
1:A:214:ASN:ND2	1:A:288:TYR:H	2.12	0.48
1:D:267:GLY:O	1:D:425:LYS:CE	2.62	0.47
1:C:89:PHE:HB3	1:C:90:PRO:HD3	1.97	0.47
1:B:214:ASN:HD21	1:B:288:TYR:H	1.62	0.47
1:B:307:ASN:HD21	1:B:468:ARG:HB2	1.79	0.47
1:C:168:TYR:CE1	1:C:471:VAL:HG23	2.49	0.47
1:A:52:LEU:HA	1:A:55:TYR:CD2	2.50	0.47
1:B:465:ILE:N	1:B:465:ILE:HD12	2.29	0.47
1:C:37:GLY:HA3	1:C:107:ILE:HG21	1.95	0.47
1:D:465:ILE:N	1:D:465:ILE:HD12	2.30	0.47
1:C:189:GLU:OE2	1:C:515:SER:HB3	2.14	0.47
1:B:220:LYS:HE2	1:B:229:PRO:O	2.14	0.46
1:A:433:ARG:NH1	1:A:435:GLN:HE22	2.13	0.46
1:B:435:GLN:HE22	1:B:480:HIS:CE1	2.33	0.46
1:B:454:LYS:HE2	6:B:740:HOH:O	2.14	0.46
1:D:274:SER:HB3	1:D:275:PRO:CD	2.45	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:THR:OG1	1:D:335:HIS:HD2	1.97	0.46
1:A:285:GLY:HA3	1:A:299:ALA:O	2.16	0.46
1:A:386:GLU:HG3	6:A:809:HOH:O	2.15	0.46
1:B:394:GLN:O	1:B:395:LEU:HD23	2.16	0.46
1:B:307:ASN:HD21	1:B:469:TRP:H	1.62	0.46
1:C:52:LEU:HD13	1:C:100:LEU:CD2	2.45	0.46
1:A:349:ASN:HD21	1:A:363:GLY:CA	2.29	0.46
1:C:233:ARG:HB3	1:C:233:ARG:NH2	2.31	0.46
1:C:429:THR:HG23	1:C:430:GLY:H	1.81	0.46
1:D:103:ALA:O	1:D:106:SER:HB2	2.15	0.46
1:A:87:VAL:HG21	1:A:341:ILE:HD13	1.99	0.45
1:C:429:THR:HG23	1:C:430:GLY:N	2.31	0.45
1:D:275:PRO:O	1:D:278:ASP:HB2	2.15	0.45
1:D:168:TYR:CE1	1:D:471:VAL:HG23	2.52	0.45
1:A:177:VAL:CG1	3:A:605:GOL:H11	2.47	0.45
1:B:307:ASN:HD21	1:B:469:TRP:N	2.14	0.45
1:C:197:HIS:CD2	3:C:602:GOL:C3	2.99	0.45
1:A:465:ILE:N	1:A:465:ILE:HD12	2.32	0.45
1:A:99:LYS:HG3	1:A:375:PHE:CD1	2.51	0.45
1:C:26:LYS:N	1:C:27:PRO:HD3	2.32	0.44
1:B:432:ASP:O	1:B:433:ARG:C	2.56	0.44
1:C:38:ILE:HD11	1:C:103:ALA:HB1	1.99	0.44
1:A:177:VAL:HG11	3:A:605:GOL:H12	2.00	0.44
1:C:197:HIS:HD2	3:C:602:GOL:C3	2.30	0.44
1:A:89:PHE:HB3	1:A:90:PRO:HD3	1.98	0.44
1:C:343:ARG:NH2	1:D:432:ASP:OD1	2.50	0.44
1:C:64:LYS:N	1:C:65:PRO:CD	2.80	0.44
1:D:327:TRP:CE3	1:D:391:ILE:HG12	2.53	0.44
1:D:307:ASN:H	1:D:307:ASN:HD22	1.66	0.44
1:C:429:THR:CG2	1:C:430:GLY:N	2.81	0.44
1:D:214:ASN:HD21	1:D:288:TYR:N	2.15	0.44
1:B:217:ALA:HB2	1:B:224:PRO:HD3	2.00	0.44
1:A:243:CYS:HA	1:A:270:THR:O	2.18	0.43
1:D:118:GLU:OE2	1:D:318:HIS:ND1	2.31	0.43
1:C:357:THR:HB	1:C:358:PRO:CD	2.49	0.43
1:B:64:LYS:N	1:B:65:PRO:CD	2.82	0.43
1:A:349:ASN:ND2	1:A:351:SER:H	2.08	0.43
1:B:7:PRO:HB2	1:B:396:GLY:O	2.19	0.43
1:C:333:THR:OG1	1:C:335:HIS:HD2	2.02	0.43
1:B:14:ARG:HH21	3:B:602:GOL:H11	1.84	0.42
1:B:252:PHE:CZ	1:B:272:VAL:HB	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:THR:HB	1:D:358:PRO:CD	2.48	0.42
1:A:274:SER:HB3	1:A:275:PRO:HD2	2.01	0.42
1:C:197:HIS:HD2	3:C:602:GOL:H2	1.83	0.42
1:C:440:PHE:CE2	1:C:465:ILE:HD13	2.54	0.42
1:C:143:GLN:HG3	1:C:143:GLN:O	2.19	0.42
1:D:336:THR:HG23	1:D:390:ASN:ND2	2.35	0.42
1:B:472:VAL:HG12	1:C:162:PRO:HB2	2.02	0.42
1:A:486:HIS:HD2	2:A:601:CIT:O6	2.02	0.42
1:A:214:ASN:HD21	1:A:288:TYR:N	2.18	0.42
1:B:170:LYS:HE2	1:B:174:TYR:CE2	2.55	0.42
1:C:484:VAL:HG11	1:D:344:ASN:ND2	2.35	0.42
1:A:28:LEU:HA	1:A:28:LEU:HD12	1.89	0.41
1:A:429:THR:HB	1:A:431:ILE:HG13	2.03	0.41
1:C:442:MET:HE1	1:C:483:ILE:CG2	2.50	0.41
1:D:448:VAL:O	1:D:455:THR:HA	2.21	0.41
1:D:489:LEU:HD22	1:D:492:MET:HE3	2.03	0.41
1:C:451:ALA:C	1:C:453:GLY:H	2.24	0.41
1:C:54:GLY:O	6:C:701:HOH:O	2.21	0.41
1:B:14:ARG:HH21	3:B:602:GOL:H12	1.85	0.41
1:B:52:LEU:HA	1:B:55:TYR:CD2	2.56	0.41
1:D:236:VAL:HG12	1:D:236:VAL:O	2.20	0.41
1:B:435:GLN:HA	1:B:435:GLN:HE21	1.85	0.41
2:A:601:CIT:O3	2:A:601:CIT:O7	2.32	0.40
1:B:77:TYR:O	1:B:468:ARG:NH1	2.53	0.40
1:B:435:GLN:CG	1:B:478:LEU:HD12	2.51	0.40
1:D:489:LEU:HD23	1:D:489:LEU:HA	1.90	0.40
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.96	0.40
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.95	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	532/549 (97%)	510 (96%)	21 (4%)	1 (0%)	47	58
1	B	529/549 (96%)	503 (95%)	21 (4%)	5 (1%)	17	20
1	C	527/549 (96%)	506 (96%)	18 (3%)	3 (1%)	25	31
1	D	526/549 (96%)	506 (96%)	20 (4%)	0	100	100
All	All	2114/2196 (96%)	2025 (96%)	80 (4%)	9 (0%)	34	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	433	ARG
1	B	477	CYS
1	B	431	ILE
1	C	452	ASN
1	C	134	GLN
1	A	450	ASP
1	B	7	PRO
1	B	478	LEU
1	C	27	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	451/462 (98%)	434 (96%)	17 (4%)	33	47
1	B	448/462 (97%)	430 (96%)	18 (4%)	31	44
1	C	446/462 (96%)	421 (94%)	25 (6%)	21	29
1	D	446/462 (96%)	432 (97%)	14 (3%)	40	55
All	All	1791/1848 (97%)	1717 (96%)	74 (4%)	30	43

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	13	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	64	LYS
1	A	149	ARG
1	A	223	SER
1	A	276	HIS
1	A	343	ARG
1	A	365	SER
1	A	369	THR
1	A	379	SER
1	A	433	ARG
1	A	435	GLN
1	A	448	VAL
1	A	482	ASP
1	A	501	LYS
1	A	518	LYS
1	A	537	LEU
1	B	143	GLN
1	B	225	THR
1	B	269	VAL
1	B	276	HIS
1	B	293	ILE
1	B	343	ARG
1	B	369	THR
1	B	419	SER
1	B	431	ILE
1	B	435	GLN
1	B	454	LYS
1	B	457	GLU
1	B	468	ARG
1	B	474	CYS
1	B	481	LEU
1	B	501	LYS
1	B	530	LYS
1	B	536	LYS
1	C	38	ILE
1	C	109	PRO
1	C	142	LYS
1	C	219	LEU
1	C	233	ARG
1	C	268	LEU
1	C	276	HIS
1	C	340	ASP
1	C	351	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	362	PRO
1	C	365	SER
1	C	369	THR
1	C	374	PRO
1	C	386	GLU
1	C	393	ARG
1	C	410	GLU
1	C	412	LYS
1	C	429	THR
1	C	448	VAL
1	C	452	ASN
1	C	454	LYS
1	C	456	ARG
1	C	474	CYS
1	C	484	VAL
1	C	495	ASP
1	D	19	ARG
1	D	100	LEU
1	D	106	SER
1	D	193	GLN
1	D	205	GLU
1	D	243	CYS
1	D	269	VAL
1	D	313	PRO
1	D	343	ARG
1	D	409	PRO
1	D	448	VAL
1	D	455	THR
1	D	468	ARG
1	D	474	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	214	ASN
1	A	265	ASN
1	A	306	ASN
1	A	307	ASN
1	A	335	HIS
1	A	349	ASN
1	A	435	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	486	HIS
1	B	56	HIS
1	B	93	HIS
1	B	214	ASN
1	B	295	GLN
1	B	306	ASN
1	B	307	ASN
1	B	319	HIS
1	B	335	HIS
1	B	344	ASN
1	B	349	ASN
1	B	373	ASN
1	B	435	GLN
1	B	480	HIS
1	B	486	HIS
1	C	56	HIS
1	C	197	HIS
1	C	214	ASN
1	C	276	HIS
1	C	306	ASN
1	C	307	ASN
1	C	319	HIS
1	C	335	HIS
1	C	349	ASN
1	C	373	ASN
1	C	486	HIS
1	D	22	ASN
1	D	56	HIS
1	D	214	ASN
1	D	248	ASN
1	D	276	HIS
1	D	306	ASN
1	D	307	ASN
1	D	335	HIS
1	D	349	ASN
1	D	373	ASN
1	D	486	HIS

### 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 ⓘ

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 for Mogul analysis.

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	$\# Z  > 2$
3	GOL	A	605	-	5,5,5	0.59	0	5,5,5	1.12	1 (20%)
3	GOL	B	605	-	5,5,5	0.53	0	5,5,5	0.50	0
3	GOL	D	602	-	5,5,5	0.71	0	5,5,5	0.86	0
3	GOL	D	605	-	5,5,5	0.86	0	5,5,5	0.55	0
3	GOL	A	604	-	5,5,5	0.38	0	5,5,5	0.55	0
3	GOL	B	602	-	5,5,5	0.62	0	5,5,5	0.87	0
3	GOL	A	602	-	5,5,5	0.41	0	5,5,5	1.38	1 (20%)
3	GOL	D	603	-	5,5,5	0.29	0	5,5,5	0.70	0
3	GOL	A	603	-	5,5,5	0.28	0	5,5,5	1.00	0
3	GOL	C	603	-	5,5,5	0.69	0	5,5,5	0.65	0
2	CIT	A	601	-	3,12,12	1.24	1 (33%)	3,17,17	4.29	2 (66%)
3	GOL	B	604	-	5,5,5	0.15	0	5,5,5	0.70	0
3	GOL	B	603	-	5,5,5	0.30	0	5,5,5	0.65	0
2	CIT	B	601	-	3,12,12	2.08	1 (33%)	3,17,17	1.41	0
3	GOL	D	604	-	5,5,5	0.49	0	5,5,5	0.43	0
2	CIT	C	601	-	3,12,12	1.62	1 (33%)	3,17,17	2.86	1 (33%)
2	CIT	D	601	-	3,12,12	2.00	1 (33%)	3,17,17	2.45	1 (33%)
3	GOL	C	602	-	5,5,5	0.50	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
3	GOL	A	605	-	-	4/4/4/4	-
3	GOL	B	605	-	-	2/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
3	GOL	D	605	-	-	2/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
3	GOL	B	602	-	-	4/4/4/4	-
3	GOL	A	602	-	-	3/4/4/4	-
3	GOL	D	603	-	-	0/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	C	603	-	-	2/4/4/4	-
2	CIT	A	601	-	-	4/6/16/16	-
3	GOL	B	604	-	-	0/4/4/4	-
3	GOL	B	603	-	-	0/4/4/4	-
2	CIT	B	601	-	-	3/6/16/16	-
3	GOL	D	604	-	-	2/4/4/4	-
2	CIT	C	601	-	-	2/6/16/16	-
2	CIT	D	601	-	-	1/6/16/16	-
3	GOL	C	602	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	CIT	C2-C3	-3.42	1.50	1.54
2	B	601	CIT	C2-C3	-3.17	1.50	1.54
2	C	601	CIT	C2-C3	-2.27	1.51	1.54
2	A	601	CIT	C4-C3	-2.03	1.52	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	CIT	C3-C4-C5	-6.83	104.05	114.98
2	C	601	CIT	C3-C4-C5	-4.68	107.49	114.98
2	D	601	CIT	C3-C2-C1	-3.95	108.66	114.98
2	A	601	CIT	C3-C2-C1	2.53	119.04	114.98
3	A	605	GOL	O1-C1-C2	2.42	121.79	110.20
3	A	602	GOL	O3-C3-C2	2.26	121.03	110.20



There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	GOL	O1-C1-C2-O2
3	A	605	GOL	O1-C1-C2-C3
3	A	605	GOL	C1-C2-C3-O3
3	A	603	GOL	O1-C1-C2-C3
3	C	603	GOL	C1-C2-C3-O3
3	C	603	GOL	O2-C2-C3-O3
3	D	604	GOL	O1-C1-C2-C3
2	A	601	CIT	C1-C2-C3-O7
2	A	601	CIT	C1-C2-C3-C4
2	A	601	CIT	C1-C2-C3-C6
3	D	602	GOL	O1-C1-C2-C3
2	B	601	CIT	C1-C2-C3-C6
3	D	605	GOL	C1-C2-C3-O3
3	D	605	GOL	O2-C2-C3-O3
3	A	604	GOL	O1-C1-C2-C3
3	A	604	GOL	C1-C2-C3-O3
2	B	601	CIT	C1-C2-C3-O7
3	D	604	GOL	O1-C1-C2-O2
2	D	601	CIT	C2-C3-C4-C5
3	B	605	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	C1-C2-C3-O3
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	C	602	GOL	O1-C1-C2-C3
3	D	602	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-O2
3	C	602	GOL	O1-C1-C2-O2
3	A	605	GOL	O2-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
2	B	601	CIT	C1-C2-C3-C4
3	A	603	GOL	O1-C1-C2-O2
3	A	604	GOL	O2-C2-C3-O3
3	B	602	GOL	O1-C1-C2-O2
2	A	601	CIT	C6-C3-C4-C5
2	C	601	CIT	C1-C2-C3-C6
3	B	605	GOL	O1-C1-C2-O2
2	C	601	CIT	C1-C2-C3-C4

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	GOL	2	0
3	D	605	GOL	1	0
3	B	602	GOL	3	0
3	A	602	GOL	9	0
2	A	601	CIT	2	0
2	B	601	CIT	1	0
2	C	601	CIT	4	0
2	D	601	CIT	4	0
3	C	602	GOL	3	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	534/549 (97%)	0.22	48 (8%) <b>9</b> <b>12</b>	25, 39, 108, 170	0
1	B	531/549 (96%)	0.21	57 (10%) <b>6</b> <b>8</b>	26, 42, 111, 159	0
1	C	529/549 (96%)	0.09	27 (5%) <b>28</b> <b>35</b>	30, 47, 83, 136	0
1	D	528/549 (96%)	0.08	28 (5%) <b>26</b> <b>33</b>	27, 46, 80, 114	0
All	All	2122/2196 (96%)	0.15	160 (7%) <b>14</b> <b>19</b>	25, 43, 91, 170	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	ILE	15.6
1	B	526	ALA	8.9
1	A	512	GLY	8.7
1	A	520	ALA	8.0
1	B	516	ALA	7.9
1	A	514	PRO	7.6
1	B	435	GLN	7.4
1	A	526	ALA	7.4
1	A	433	ARG	6.8
1	A	522	ASP	6.8
1	B	477	CYS	6.7
1	A	513	VAL	6.5
1	C	409	PRO	6.4
1	B	431	ILE	6.4
1	B	525	SER	6.3
1	B	225	THR	6.0
1	C	226	PRO	5.9
1	C	451	ALA	5.9
1	D	228	ASP	5.9
1	B	517	ALA	5.8
1	A	477	CYS	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	518	LYS	5.7
1	D	409	PRO	5.7
1	B	6	ALA	5.7
1	B	227	GLY	5.4
1	A	227	GLY	5.4
1	B	518	LYS	5.4
1	A	431	ILE	5.3
1	B	228	ASP	5.1
1	A	517	ALA	5.0
1	B	451	ALA	4.9
1	A	516	ALA	4.9
1	A	432	ASP	4.6
1	A	434	ALA	4.6
1	B	226	PRO	4.5
1	A	525	SER	4.5
1	D	410	GLU	4.4
1	B	433	ARG	4.4
1	A	226	PRO	4.4
1	A	515	SER	4.4
1	D	451	ALA	4.4
1	B	522	ASP	4.3
1	C	452	ASN	4.3
1	B	514	PRO	4.3
1	A	527	LEU	4.3
1	B	479	THR	4.2
1	C	227	GLY	4.2
1	C	142	LYS	4.2
1	D	140	ASP	4.1
1	B	223	SER	4.1
1	C	6	ALA	4.0
1	D	226	PRO	4.0
1	A	228	ASP	4.0
1	A	519	ALA	4.0
1	D	141	GLY	3.9
1	C	228	ASP	3.9
1	B	292	GLU	3.8
1	A	225	THR	3.7
1	B	520	ALA	3.7
1	B	293	ILE	3.7
1	B	291	ASP	3.7
1	B	519	ALA	3.7
1	D	453	GLY	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	452	ASN	3.6
1	D	378	ALA	3.5
1	A	322	VAL	3.5
1	B	378	ALA	3.4
1	A	481	LEU	3.4
1	C	141	GLY	3.3
1	B	521	ILE	3.3
1	C	225	THR	3.3
1	C	413	SER	3.3
1	A	523	LYS	3.3
1	D	418	PRO	3.2
1	A	229	PRO	3.2
1	B	510	GLY	3.2
1	A	524	VAL	3.2
1	B	279	ILE	3.1
1	B	432	ASP	3.1
1	B	527	LEU	3.1
1	D	229	PRO	3.1
1	B	478	LEU	3.1
1	A	452	ASN	3.0
1	C	143	GLN	3.0
1	B	434	ALA	3.0
1	C	22	ASN	3.0
1	B	524	VAL	3.0
1	B	141	GLY	2.9
1	A	379	SER	2.9
1	C	322	VAL	2.9
1	B	523	LYS	2.9
1	B	22	ASN	2.9
1	B	407	ALA	2.9
1	D	433	ARG	2.9
1	B	224	PRO	2.9
1	A	528	GLN	2.8
1	D	322	VAL	2.8
1	A	453	GLY	2.8
1	B	528	GLN	2.8
1	C	315	PHE	2.8
1	D	142	LYS	2.8
1	B	513	VAL	2.8
1	D	317	PHE	2.7
1	C	23	GLY	2.7
1	D	227	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	338	ARG	2.7
1	D	454	LYS	2.7
1	A	291	ASP	2.7
1	A	224	PRO	2.7
1	A	314	ILE	2.6
1	A	381	GLU	2.6
1	C	338	ARG	2.6
1	B	322	VAL	2.6
1	B	314	ILE	2.6
1	B	140	ASP	2.6
1	B	452	ASN	2.6
1	A	480	HIS	2.6
1	A	478	LEU	2.5
1	B	142	LYS	2.5
1	C	476	ASN	2.5
1	D	419	SER	2.5
1	C	140	ASP	2.5
1	A	479	THR	2.5
1	A	435	GLN	2.5
1	D	139	LEU	2.5
1	C	44	SER	2.4
1	D	316	PHE	2.4
1	A	22	ASN	2.4
1	D	496	ASP	2.4
1	C	97	VAL	2.4
1	A	451	ALA	2.4
1	B	379	SER	2.3
1	C	317	PHE	2.3
1	D	412	LYS	2.3
1	A	317	PHE	2.3
1	B	409	PRO	2.3
1	C	408	THR	2.3
1	B	381	GLU	2.3
1	D	519	ALA	2.3
1	D	314	ILE	2.3
1	B	318	HIS	2.2
1	A	205	GLU	2.2
1	B	317	PHE	2.2
1	B	476	ASN	2.2
1	A	409	PRO	2.2
1	A	97	VAL	2.2
1	B	316	PHE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	2.1
1	D	476	ASN	2.1
1	B	275	PRO	2.1
1	A	279	ILE	2.1
1	C	316	PHE	2.1
1	C	450	ASP	2.0
1	C	410	GLU	2.0
1	B	116	TRP	2.0
1	A	141	GLY	2.0
1	B	515	SER	2.0
1	C	475	ALA	2.0
1	B	319	HIS	2.0
1	D	413	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 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
3	GOL	A	604	6/6	0.78	0.23	69,77,80,81	0
3	GOL	D	605	6/6	0.79	0.25	57,65,70,71	0
3	GOL	C	602	6/6	0.83	0.14	69,72,77,86	0
3	GOL	D	604	6/6	0.87	0.28	57,69,75,75	0
3	GOL	A	605	6/6	0.87	0.43	59,66,69,74	0
3	GOL	B	604	6/6	0.88	0.13	64,67,78,80	0
3	GOL	C	603	6/6	0.89	0.20	54,69,72,73	0
3	GOL	A	603	6/6	0.89	0.20	52,69,77,79	0
3	GOL	D	603	6/6	0.92	0.17	55,63,67,69	0
3	GOL	D	602	6/6	0.92	0.16	50,58,62,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	602	6/6	0.92	0.09	54,61,64,64	0
3	GOL	B	605	6/6	0.93	0.19	53,62,68,74	0
3	GOL	B	603	6/6	0.93	0.14	58,63,64,72	0
2	CIT	B	601	13/13	0.93	0.16	34,55,67,70	0
2	CIT	C	601	13/13	0.94	0.15	50,56,63,64	0
2	CIT	D	601	13/13	0.94	0.14	47,55,60,60	0
5	O	B	608	1/1	0.95	0.24	25,25,25,25	0
2	CIT	A	601	13/13	0.95	0.12	33,51,60,61	0
3	GOL	A	602	6/6	0.96	0.10	47,50,52,52	0
4	CU	B	606	1/1	0.98	0.13	47,47,47,47	0
5	O	C	606	1/1	0.98	0.25	28,28,28,28	0
5	O	D	608	1/1	0.98	0.23	34,34,34,34	0
5	O	A	608	1/1	0.98	0.18	25,25,25,25	0
4	CU	C	604	1/1	0.99	0.14	54,54,54,54	0
4	CU	B	607	1/1	0.99	0.12	36,36,36,36	0
4	CU	A	607	1/1	0.99	0.10	45,45,45,45	0
4	CU	D	606	1/1	1.00	0.14	40,40,40,40	0
4	CU	A	606	1/1	1.00	0.11	33,33,33,33	0
4	CU	C	605	1/1	1.00	0.13	42,42,42,42	0
4	CU	D	607	1/1	1.00	0.15	51,51,51,51	0

## 6.5 Other polymers

There are no such residues in this entry.