



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 07:29 AM EDT

PDB ID : 3GG2  
Title : Crystal structure of UDP-glucose 6-dehydrogenase from *Porphyromonas gingivalis* bound to product UDP-glucuronate  
Authors : Bonanno, J.B.; Freeman, J.; Bain, K.T.; Chang, S.; Sampathkumar, P.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : unknown  
Resolution : 1.70 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

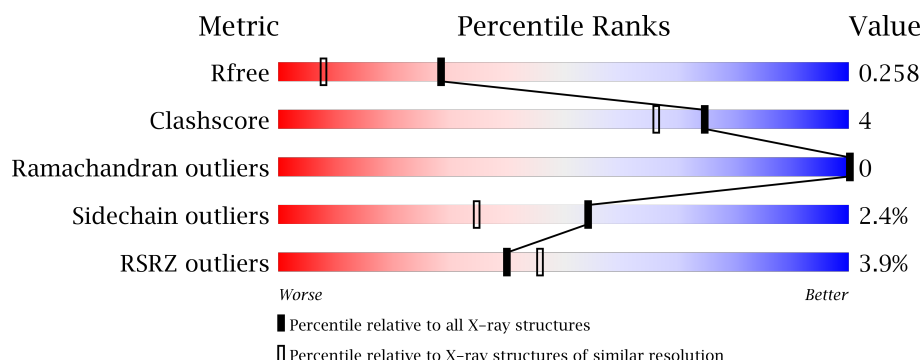
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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. 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	450	<div> <div>3%</div> <div>87%</div> <div>8%</div> <div>• •</div> </div>
1	B	450	<div> <div>6%</div> <div>84%</div> <div>9%</div> <div>• 6%</div> </div>
1	C	450	<div> <div>3%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	D	450	<div> <div>2%</div> <div>88%</div> <div>6%</div> <div>• 5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14679 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 Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	8	0
			3360	2136	570	631	23			
1	B	425	Total	C	N	O	S	0	2	0
			3256	2065	551	617	23			
1	C	420	Total	C	N	O	S	0	3	0
			3229	2048	545	613	23			
1	D	427	Total	C	N	O	S	0	4	0
			3305	2101	561	620	23			

There are 60 discrepancies between the modelled and reference sequences:

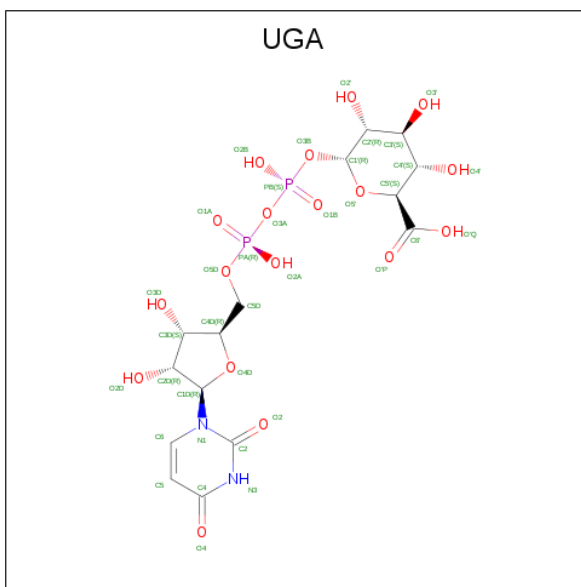
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	expression tag	UNP Q7MVC7
A	78	SER	-	expression tag	UNP Q7MVC7
A	79	LEU	-	expression tag	UNP Q7MVC7
A	158	ILE	VAL	engineered	UNP Q7MVC7
A	175	SER	GLY	engineered	UNP Q7MVC7
A	211	ALA	VAL	engineered	UNP Q7MVC7
A	485	ALA	THR	engineered	UNP Q7MVC7
A	519	GLU	-	expression tag	UNP Q7MVC7
A	520	GLY	-	expression tag	UNP Q7MVC7
A	521	HIS	-	expression tag	UNP Q7MVC7
A	522	HIS	-	expression tag	UNP Q7MVC7
A	523	HIS	-	expression tag	UNP Q7MVC7
A	524	HIS	-	expression tag	UNP Q7MVC7
A	525	HIS	-	expression tag	UNP Q7MVC7
A	526	HIS	-	expression tag	UNP Q7MVC7
B	77	MET	-	expression tag	UNP Q7MVC7
B	78	SER	-	expression tag	UNP Q7MVC7
B	79	LEU	-	expression tag	UNP Q7MVC7
B	158	ILE	VAL	engineered	UNP Q7MVC7
B	175	SER	GLY	engineered	UNP Q7MVC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ALA	VAL	engineered	UNP Q7MVC7
B	485	ALA	THR	engineered	UNP Q7MVC7
B	519	GLU	-	expression tag	UNP Q7MVC7
B	520	GLY	-	expression tag	UNP Q7MVC7
B	521	HIS	-	expression tag	UNP Q7MVC7
B	522	HIS	-	expression tag	UNP Q7MVC7
B	523	HIS	-	expression tag	UNP Q7MVC7
B	524	HIS	-	expression tag	UNP Q7MVC7
B	525	HIS	-	expression tag	UNP Q7MVC7
B	526	HIS	-	expression tag	UNP Q7MVC7
C	77	MET	-	expression tag	UNP Q7MVC7
C	78	SER	-	expression tag	UNP Q7MVC7
C	79	LEU	-	expression tag	UNP Q7MVC7
C	158	ILE	VAL	engineered	UNP Q7MVC7
C	175	SER	GLY	engineered	UNP Q7MVC7
C	211	ALA	VAL	engineered	UNP Q7MVC7
C	485	ALA	THR	engineered	UNP Q7MVC7
C	519	GLU	-	expression tag	UNP Q7MVC7
C	520	GLY	-	expression tag	UNP Q7MVC7
C	521	HIS	-	expression tag	UNP Q7MVC7
C	522	HIS	-	expression tag	UNP Q7MVC7
C	523	HIS	-	expression tag	UNP Q7MVC7
C	524	HIS	-	expression tag	UNP Q7MVC7
C	525	HIS	-	expression tag	UNP Q7MVC7
C	526	HIS	-	expression tag	UNP Q7MVC7
D	77	MET	-	expression tag	UNP Q7MVC7
D	78	SER	-	expression tag	UNP Q7MVC7
D	79	LEU	-	expression tag	UNP Q7MVC7
D	158	ILE	VAL	engineered	UNP Q7MVC7
D	175	SER	GLY	engineered	UNP Q7MVC7
D	211	ALA	VAL	engineered	UNP Q7MVC7
D	485	ALA	THR	engineered	UNP Q7MVC7
D	519	GLU	-	expression tag	UNP Q7MVC7
D	520	GLY	-	expression tag	UNP Q7MVC7
D	521	HIS	-	expression tag	UNP Q7MVC7
D	522	HIS	-	expression tag	UNP Q7MVC7
D	523	HIS	-	expression tag	UNP Q7MVC7
D	524	HIS	-	expression tag	UNP Q7MVC7
D	525	HIS	-	expression tag	UNP Q7MVC7
D	526	HIS	-	expression tag	UNP Q7MVC7

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O<sub>18</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	A	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	B	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	C	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	D	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	D	1	Total 37	C 15	N 2	O 18	P 2	0	0

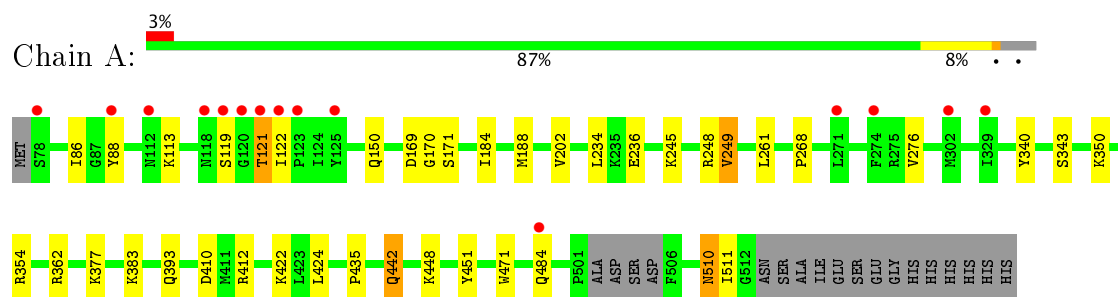
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	362	Total O 362 362	0	0
3	B	295	Total O 295 295	0	0
3	C	366	Total O 366 366	0	0
3	D	284	Total O 284 284	0	0

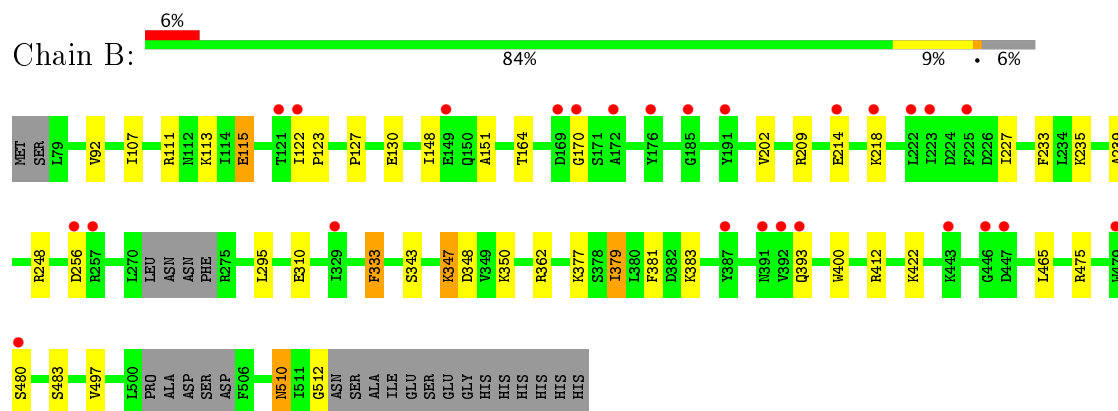
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

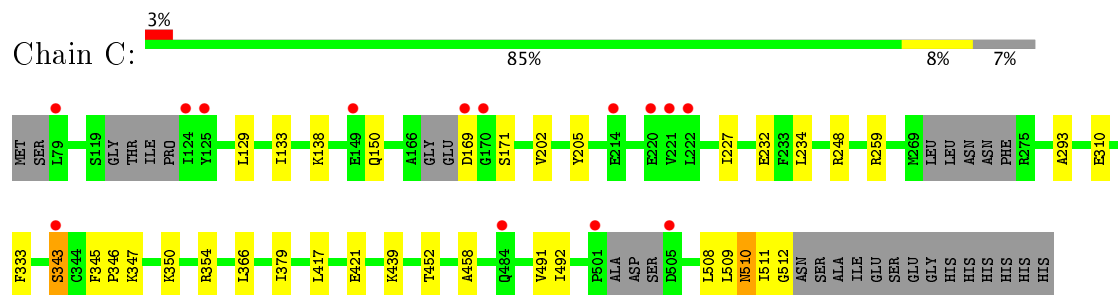
- Molecule 1: Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family



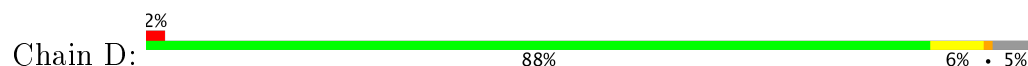
- Molecule 1: Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family

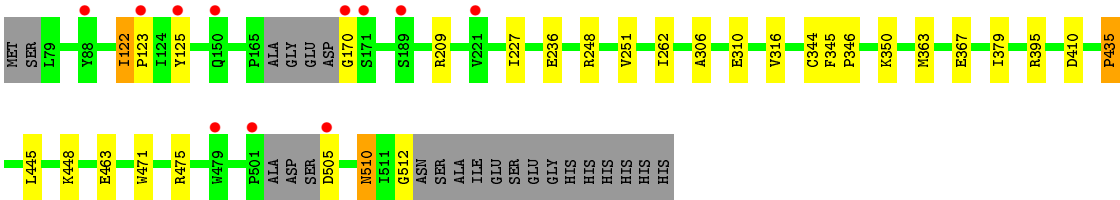


- Molecule 1: Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family



- Molecule 1: Sugar dehydrogenase, UDP-glucose/GDP-mannose dehydrogenase family





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.36 Å 143.49 Å 85.50 Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 44.35 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-1.70) 93.3 (44.35-1.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 1.70 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.215 , 0.256 0.218 , 0.258	Depositor DCC
$R_{free}$ test set	9459 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: UGA

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	0/3438	0.76	0/4642
1	B	0.67	0/3312	0.72	1/4476 (0.0%)
1	C	0.70	0/3286	0.74	0/4438
1	D	0.70	0/3370	0.73	1/4553 (0.0%)
All	All	0.71	0/13406	0.74	2/18109 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344	CYS	CA-CB-SG	-5.43	104.23	114.00
1	B	377	LYS	CD-CE-NZ	5.01	123.21	111.70

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	3360	0	3402	29	0
1	B	3256	0	3256	29	1
1	C	3229	0	3222	23	0
1	D	3305	0	3322	17	0
2	A	74	0	38	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	37	0	19	0	0
2	C	37	0	19	0	0
2	D	74	0	38	1	0
3	A	362	0	0	4	0
3	B	295	0	0	4	0
3	C	366	0	0	5	0
3	D	284	0	0	1	1
All	All	14679	0	13316	98	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 4.

All (98) 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:448:LYS:HG3	3:A:1815:HOH:O	1.65	0.94
1:C:202:VAL:HG23	3:C:560:HOH:O	1.74	0.87
1:B:107:ILE:HD11	1:B:151:ALA:HB2	1.61	0.82
1:B:107:ILE:HD11	1:B:151:ALA:CB	2.10	0.81
1:B:233:PHE:O	3:B:2215:HOH:O	2.02	0.78
1:A:86:ILE:HD12	1:A:113:LYS:HD3	1.65	0.77
1:C:232[A]:GLU:CG	1:C:234:LEU:HG	2.16	0.75
1:C:439:LYS:HG3	3:C:33:HOH:O	1.89	0.72
1:A:170:GLY:HA3	1:A:350:LYS:HE2	1.74	0.70
1:B:113:LYS:HD2	1:B:123:PRO:HB3	1.75	0.69
1:A:249[A]:VAL:HG13	1:A:276:VAL:HA	1.75	0.68
1:C:343:SER:O	1:C:347:LYS:HG2	1.95	0.67
1:B:310:GLU:HG3	1:B:512:GLY:HA2	1.78	0.66
1:A:383:LYS:HE3	1:A:511:ILE:HD13	1.78	0.66
1:D:445:LEU:O	1:D:448:LYS:HG2	1.99	0.63
1:B:475:ARG:HD3	1:B:497:VAL:HG11	1.80	0.62
1:B:379:ILE:O	1:B:383:LYS:HG2	2.00	0.62
1:C:232[A]:GLU:HG3	1:C:234:LEU:HG	1.80	0.62
1:C:171:SER:HB3	1:C:354:ARG:HG2	1.82	0.61
1:D:209:ARG:HB2	1:D:227:ILE:HD13	1.83	0.60
1:B:209:ARG:HB2	1:B:227:ILE:HD13	1.84	0.60
1:B:113:LYS:HD2	1:B:123:PRO:CB	2.33	0.57
1:B:202:VAL:HG23	3:B:1220:HOH:O	2.04	0.56
1:A:119:SER:HB2	1:A:121:THR:HG22	1.88	0.56
1:A:249[A]:VAL:CG1	1:A:276:VAL:HG22	2.36	0.56
1:A:88[B]:TYR:HD1	1:A:234:LEU:HD11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:LYS:HG3	3:C:540:HOH:O	2.06	0.55
1:B:343:SER:OG	1:B:412:ARG:NE	2.39	0.55
1:B:107:ILE:HD13	1:B:148:ILE:HA	1.89	0.55
1:B:164:THR:O	1:B:347:LYS:HE3	2.07	0.54
1:A:86:ILE:CD1	1:A:113:LYS:HD3	2.35	0.53
1:C:510:ASN:HD22	1:C:510:ASN:C	2.11	0.52
1:C:232[A]:GLU:HG2	1:C:234:LEU:HG	1.89	0.50
1:B:343:SER:OG	1:B:412:ARG:CZ	2.60	0.50
1:C:417:LEU:O	1:C:421:GLU:HG2	2.12	0.50
1:A:249[A]:VAL:HG11	1:A:276:VAL:HG22	1.94	0.49
1:D:510:ASN:C	1:D:510:ASN:HD22	2.15	0.49
1:A:442:GLN:NE2	3:A:815:HOH:O	2.39	0.49
1:A:113:LYS:HE2	1:A:122:ILE:HD13	1.94	0.49
1:B:381:PHE:CG	1:B:422:LYS:HG3	2.47	0.48
1:A:171:SER:HB3	1:A:354:ARG:HG2	1.94	0.48
1:A:88[B]:TYR:CD1	1:A:234:LEU:HD11	2.49	0.47
1:C:259:ARG:NH1	3:C:2896:HOH:O	2.39	0.47
1:D:435:PRO:HG2	1:D:471:TRP:CD2	2.49	0.47
1:B:113:LYS:HD3	3:B:1759:HOH:O	2.13	0.47
1:B:347:LYS:HE2	1:B:348:ASP:OD1	2.15	0.47
1:B:510:ASN:C	1:B:510:ASN:HD22	2.18	0.47
1:C:492:ILE:HG12	1:C:509:LEU:HD12	1.97	0.47
1:D:345:PHE:HB2	1:D:346:PRO:HD3	1.97	0.46
1:D:251:VAL:HG21	1:D:262:ILE:HG21	1.97	0.46
1:A:121:THR:OG1	1:A:121:THR:O	2.34	0.46
1:B:381:PHE:CD1	1:B:422:LYS:HG3	2.51	0.45
1:A:424:LEU:HD13	1:A:448:LYS:HE2	1.98	0.45
1:C:345:PHE:HB2	1:C:346:PRO:HD3	1.97	0.45
1:D:310:GLU:HG3	1:D:512:GLY:HA2	1.98	0.45
1:B:111:ARG:O	1:B:115:GLU:HB2	2.17	0.45
1:D:395:ARG:NH1	1:D:463:GLU:OE1	2.46	0.45
1:B:170:GLY:HA3	1:B:350:LYS:HE3	1.99	0.45
1:C:205:TYR:HB2	1:C:227:ILE:HD12	1.99	0.45
1:B:122:ILE:HG23	1:B:130:GLU:HG3	1.99	0.44
1:B:475:ARG:CD	1:B:497:VAL:HG11	2.47	0.44
1:D:122:ILE:HG13	1:D:123:PRO:HD2	1.99	0.44
1:C:343:SER:OG	3:C:692:HOH:O	2.20	0.44
1:A:169:ASP:CB	3:A:1763:HOH:O	2.66	0.44
1:C:491:VAL:HG13	1:C:508:LEU:HD12	2.00	0.44
1:C:169:ASP:OD2	1:C:354:ARG:NH1	2.50	0.43
1:A:510:ASN:HD22	1:A:510:ASN:C	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ILE:HG21	1:C:511:ILE:HD13	1.99	0.43
1:D:306:ALA:HB2	1:D:316:VAL:HG21	2.01	0.43
2:A:6000:UGA:O3D	2:D:4000:UGA:H2A1	2.18	0.43
1:C:491:VAL:HG13	1:C:508:LEU:CD1	2.49	0.43
1:C:310:GLU:HG3	1:C:512:GLY:HA2	2.00	0.43
1:A:184:ILE:O	1:A:188:MET:HG3	2.19	0.42
1:A:202:VAL:HG23	3:A:1099:HOH:O	2.19	0.42
1:A:245:LYS:HZ2	2:A:6000:UGA:H5'1	1.83	0.42
1:A:268:PRO:HB3	1:D:475:ARG:HG3	2.01	0.42
1:A:245:LYS:HB3	1:A:245:LYS:HE3	1.75	0.42
1:A:249[A]:VAL:HG13	1:A:276:VAL:HG22	2.01	0.42
1:A:435:PRO:HG2	1:A:471:TRP:CD2	2.53	0.42
1:B:295:LEU:HB3	1:B:333:PHE:CE2	2.54	0.42
1:A:343:SER:HB3	1:A:412:ARG:HD2	2.00	0.42
1:B:400:TRP:CG	1:B:465:LEU:HD11	2.55	0.42
1:D:363:MET:O	1:D:367:GLU:HG3	2.20	0.42
1:D:379:ILE:HD13	3:D:574:HOH:O	2.19	0.42
1:C:452:THR:HG21	1:C:458:ALA:HA	2.02	0.42
1:D:236:GLU:OE2	1:D:410:ASP:OD2	2.37	0.42
1:B:214:GLU:O	1:B:218:LYS:HG3	2.20	0.41
1:B:235:LYS:HB2	1:B:235:LYS:HE2	1.84	0.41
1:B:92:VAL:HG21	1:B:239:ALA:HB3	2.02	0.41
1:A:236:GLU:OE2	1:A:410:ASP:OD2	2.39	0.41
1:A:442:GLN:HA	1:A:451:TYR:OH	2.20	0.41
1:B:347:LYS:HE3	3:B:618:HOH:O	2.20	0.41
1:C:293:ALA:HB1	1:C:366:LEU:HD21	2.03	0.41
1:A:340:TYR:O	1:A:377[A]:LYS:HE3	2.21	0.41
1:D:170:GLY:HA3	1:D:350:LYS:HG3	2.03	0.41
1:C:129:LEU:O	1:C:133:ILE:HG13	2.22	0.40
1:D:310:GLU:CG	1:D:512:GLY:HA2	2.52	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)
1:B:362:ARG:NH2	3:D:1429:HOH:O[1_655]	2.13	0.07

## 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	435/450 (97%)	430 (99%)	5 (1%)	0	100	100
1	B	421/450 (94%)	416 (99%)	5 (1%)	0	100	100
1	C	413/450 (92%)	406 (98%)	7 (2%)	0	100	100
1	D	425/450 (94%)	419 (99%)	6 (1%)	0	100	100
All	All	1694/1800 (94%)	1671 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	360/374 (96%)	348 (97%)	12 (3%)	43	21
1	B	343/374 (92%)	332 (97%)	11 (3%)	44	22
1	C	341/374 (91%)	335 (98%)	6 (2%)	64	47
1	D	351/374 (94%)	346 (99%)	5 (1%)	71	58
All	All	1395/1496 (93%)	1361 (98%)	34 (2%)	54	35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	A	150	GLN

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Mol	Chain	Res	Type
1	A	248	ARG
1	A	249[A]	VAL
1	A	249[B]	VAL
1	A	261	LEU
1	A	362	ARG
1	A	393	GLN
1	A	422	LYS
1	A	442	GLN
1	A	484	GLN
1	A	510	ASN
1	B	115	GLU
1	B	127	PRO
1	B	248	ARG
1	B	256	ASP
1	B	333	PHE
1	B	347	LYS
1	B	379	ILE
1	B	393	GLN
1	B	480	SER
1	B	483	SER
1	B	510	ASN
1	C	138	LYS
1	C	150	GLN
1	C	248	ARG
1	C	333	PHE
1	C	343	SER
1	C	510	ASN
1	D	122	ILE
1	D	248	ARG
1	D	435	PRO
1	D	505	ASP
1	D	510	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	510	ASN
1	B	510	ASN
1	C	150	GLN
1	C	510	ASN
1	D	510	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	UGA	A	1000	-	32,39,39	2.15	3 (9%)	44,60,60	2.22	7 (15%)
2	UGA	A	6000	-	32,39,39	2.27	3 (9%)	44,60,60	1.96	5 (11%)
2	UGA	B	2000	-	32,39,39	2.08	3 (9%)	44,60,60	2.21	7 (15%)
2	UGA	C	3000	-	32,39,39	1.97	3 (9%)	44,60,60	2.34	9 (20%)
2	UGA	D	4000	-	32,39,39	2.31	5 (15%)	44,60,60	2.02	5 (11%)
2	UGA	D	5000	-	32,39,39	2.31	3 (9%)	44,60,60	1.94	4 (9%)

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	UGA	A	1000	-	-	0/21/61/61	0/3/3/3
2	UGA	A	6000	-	-	0/21/61/61	0/3/3/3
2	UGA	B	2000	-	-	0/21/61/61	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UGA	C	3000	-	-	0/21/61/61	0/3/3/3
2	UGA	D	4000	-	-	0/21/61/61	0/3/3/3
2	UGA	D	5000	-	-	0/21/61/61	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5000	UGA	C6-N1	-9.72	1.34	1.47
2	A	6000	UGA	C6-N1	-9.04	1.35	1.47
2	D	4000	UGA	C6-N1	-8.28	1.36	1.47
2	D	4000	UGA	C6-C5	-7.71	1.38	1.52
2	C	3000	UGA	C6-N1	-7.66	1.37	1.47
2	A	1000	UGA	C6-C5	-7.46	1.38	1.52
2	B	2000	UGA	C6-N1	-7.37	1.37	1.47
2	A	1000	UGA	C6-N1	-7.14	1.38	1.47
2	A	6000	UGA	C6-C5	-7.10	1.39	1.52
2	B	2000	UGA	C6-C5	-6.70	1.40	1.52
2	D	5000	UGA	C6-C5	-6.60	1.40	1.52
2	C	3000	UGA	C6-C5	-5.95	1.41	1.52
2	B	2000	UGA	C5-C4	-4.45	1.39	1.50
2	A	1000	UGA	C5-C4	-4.40	1.39	1.50
2	A	6000	UGA	C5-C4	-4.30	1.39	1.50
2	D	5000	UGA	C5-C4	-4.09	1.40	1.50
2	D	4000	UGA	C5-C4	-4.05	1.40	1.50
2	C	3000	UGA	C5-C4	-3.68	1.41	1.50
2	D	4000	UGA	O5'-C5'	-2.14	1.41	1.44
2	D	4000	UGA	O3D-C3D	2.04	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	UGA	C4-N3-C2	-7.54	119.35	125.81
2	A	1000	UGA	C4-N3-C2	-6.59	120.16	125.81
2	A	6000	UGA	C4-N3-C2	-6.18	120.51	125.81
2	B	2000	UGA	C4-N3-C2	-5.51	121.09	125.81
2	D	4000	UGA	C4-N3-C2	-5.25	121.31	125.81
2	D	5000	UGA	C4-N3-C2	-4.44	122.00	125.81
2	A	1000	UGA	C6'-C5'-C4'	-3.64	103.56	112.98
2	A	1000	UGA	O5'-C1'-O3B	-3.10	107.31	111.36
2	B	2000	UGA	C4'-C3'-C2'	-2.95	105.63	110.84
2	C	3000	UGA	C6'-C5'-C4'	-2.59	106.27	112.98
2	C	3000	UGA	O2-C2-N3	-2.53	116.72	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	UGA	O3D-C3D-C4D	-2.51	103.75	111.09
2	B	2000	UGA	C6'-C5'-C4'	-2.42	106.70	112.98
2	C	3000	UGA	C4'-C3'-C2'	-2.21	106.93	110.84
2	A	1000	UGA	O2-C2-N3	-2.10	117.53	121.50
2	D	4000	UGA	O2A-PA-O1A	2.06	122.92	112.28
2	A	6000	UGA	C3'-C4'-C5'	2.42	113.75	108.89
2	D	5000	UGA	C5-C4-N3	2.71	119.41	116.72
2	D	5000	UGA	N3-C2-N1	2.80	119.52	116.73
2	B	2000	UGA	O3A-PB-O3B	2.87	107.19	102.05
2	A	6000	UGA	N3-C2-N1	3.17	119.89	116.73
2	A	6000	UGA	C5-C4-N3	3.27	119.97	116.72
2	D	4000	UGA	N3-C2-N1	3.29	120.01	116.73
2	D	4000	UGA	C5-C4-N3	3.35	120.05	116.72
2	A	1000	UGA	N3-C2-N1	3.41	120.13	116.73
2	C	3000	UGA	O3A-PB-O3B	3.92	109.06	102.05
2	B	2000	UGA	N3-C2-N1	3.94	120.65	116.73
2	B	2000	UGA	C5-C4-N3	4.32	121.01	116.72
2	C	3000	UGA	C5-C4-N3	4.75	121.44	116.72
2	A	1000	UGA	C5-C4-N3	4.88	121.57	116.72
2	C	3000	UGA	N3-C2-N1	5.25	121.96	116.73
2	C	3000	UGA	C5-C6-N1	8.11	119.13	110.70
2	A	1000	UGA	C5-C6-N1	8.41	119.44	110.70
2	A	6000	UGA	C5-C6-N1	8.45	119.49	110.70
2	B	2000	UGA	C5-C6-N1	9.54	120.62	110.70
2	D	5000	UGA	C5-C6-N1	9.56	120.63	110.70
2	D	4000	UGA	C5-C6-N1	9.60	120.68	110.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6000	UGA	2	0
2	D	4000	UGA	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	431/450 (95%)	0.36	15 (3%)	44 50	16, 23, 35, 41	0
1	B	425/450 (94%)	0.61	26 (6%)	22 25	17, 30, 42, 47	0
1	C	420/450 (93%)	0.39	14 (3%)	47 53	17, 27, 38, 44	0
1	D	427/450 (94%)	0.30	11 (2%)	56 62	16, 24, 36, 43	0
All	All	1703/1800 (94%)	0.41	66 (3%)	40 46	16, 26, 39, 47	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	125[A]	TYR	5.2
1	A	123	PRO	5.0
1	B	446	GLY	4.5
1	C	124	ILE	4.2
1	D	505	ASP	3.6
1	D	170	GLY	3.6
1	B	479	TRP	3.5
1	A	122	ILE	3.4
1	A	78	SER	3.3
1	A	121	THR	3.3
1	B	170	GLY	3.3
1	D	221	VAL	3.2
1	B	176	TYR	3.2
1	A	271	LEU	3.1
1	B	169	ASP	3.1
1	A	119	SER	3.1
1	B	191	TYR	3.0
1	A	88[A]	TYR	3.0
1	D	171	SER	3.0
1	B	392	VAL	3.0
1	B	480	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	218	LYS	2.8
1	B	223	ILE	2.7
1	C	505	ASP	2.7
1	A	125	TYR	2.7
1	B	391	ASN	2.7
1	D	501	PRO	2.7
1	B	121	THR	2.6
1	B	256	ASP	2.6
1	C	484	GLN	2.5
1	A	118	ASN	2.5
1	C	222	LEU	2.5
1	B	387	TYR	2.5
1	B	443	LYS	2.5
1	C	220	GLU	2.4
1	B	393	GLN	2.4
1	B	172	ALA	2.4
1	A	274	PHE	2.3
1	B	225	PHE	2.3
1	C	214	GLU	2.3
1	B	185	GLY	2.3
1	D	189	SER	2.3
1	C	170	GLY	2.2
1	C	149	GLU	2.2
1	A	120	GLY	2.2
1	B	222	LEU	2.2
1	B	329	ILE	2.2
1	A	112	ASN	2.2
1	C	125	TYR	2.2
1	A	302	MET	2.1
1	D	150	GLN	2.1
1	B	257	ARG	2.1
1	B	447	ASP	2.1
1	B	149	GLU	2.1
1	D	123	PRO	2.1
1	A	329	ILE	2.1
1	C	79	LEU	2.1
1	B	214	GLU	2.1
1	B	122	ILE	2.1
1	C	343	SER	2.1
1	A	484	GLN	2.0
1	C	221	VAL	2.0
1	D	479	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	169	ASP	2.0
1	C	501	PRO	2.0
1	D	88	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	UGA	A	6000	37/37	0.86	0.16	1.15	30,36,44,46	0
2	UGA	D	4000	37/37	0.97	0.09	-0.54	16,19,24,27	0
2	UGA	A	1000	37/37	0.97	0.10	-0.77	12,18,22,25	0
2	UGA	D	5000	37/37	0.92	0.11	-0.77	25,29,35,39	0
2	UGA	B	2000	37/37	0.96	0.09	-1.17	17,22,26,28	0
2	UGA	C	3000	37/37	0.97	0.09	-1.23	17,21,24,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.