Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 08:40 PM EST

PDB ID	:	4R7P
Title	:	Human UDP-glucose pyrophosphorylase isoform 1 in complex with UDP-glucose
Authors	:	Fuehring, J.; Cramer, J.T.; Schneider, J.; Baruch, P.; Gerardy-Schahn, R.; Fedorov, R.
Deposited on	:	2014-08-28
Resolution	:	3.35 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

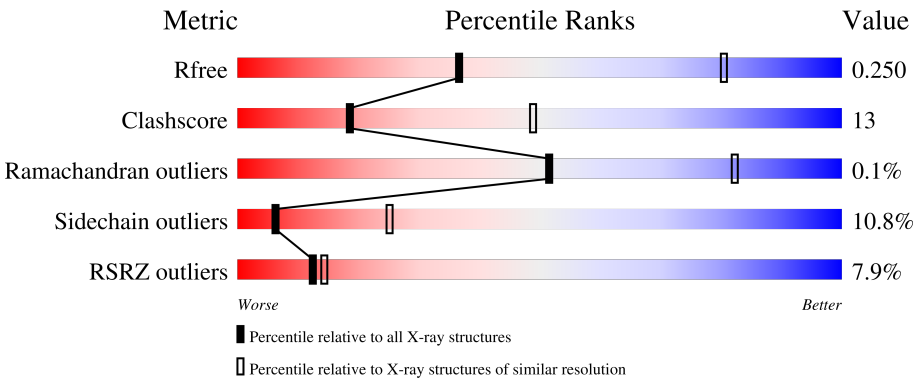
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	526	.% 64% 24% • 8%
1	B	526	2% 72% 18% • 8%
1	C	526	7% 67% 19% 6% 8%
1	D	526	19% 63% 22% 6% 9%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UPG	A	601	-	-	-	X
3	SO4	A	607	-	-	-	X
3	SO4	D	602	-	-	-	X
3	SO4	D	603	-	-	-	X
4	ACT	D	605	-	-	-	X
5	EDO	A	610	-	-	-	X
5	EDO	B	606	-	-	-	X
5	EDO	C	605	-	-	-	X
6	ZN	B	610	-	-	-	X
6	ZN	C	606	-	-	-	X
6	ZN	D	607	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15591 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 UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	485	3831	2437	658	725	11	0	0	0
1	B	485	3831	2437	658	725	11	0	0	0
1	C	485	3831	2437	658	725	11	0	0	0
1	D	480	3799	2417	653	718	11	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q16851
A	-16	ALA	-	expression tag	UNP Q16851
A	-15	SER	-	expression tag	UNP Q16851
A	-14	TRP	-	expression tag	UNP Q16851
A	-13	SER	-	expression tag	UNP Q16851
A	-12	HIS	-	expression tag	UNP Q16851
A	-11	PRO	-	expression tag	UNP Q16851
A	-10	GLN	-	expression tag	UNP Q16851
A	-9	PHE	-	expression tag	UNP Q16851
A	-8	GLU	-	expression tag	UNP Q16851
A	-7	LYS	-	expression tag	UNP Q16851
A	-6	GLY	-	expression tag	UNP Q16851
A	-5	ALA	-	expression tag	UNP Q16851
A	-4	LEU	-	expression tag	UNP Q16851
A	-3	VAL	-	expression tag	UNP Q16851
A	-2	PRO	-	expression tag	UNP Q16851
A	-1	ARG	-	expression tag	UNP Q16851
A	0	GLY	-	expression tag	UNP Q16851
A	1	SER	-	expression tag	UNP Q16851
B	-17	MET	-	expression tag	UNP Q16851
B	-16	ALA	-	expression tag	UNP Q16851

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	SER	-	expression tag	UNP Q16851
B	-14	TRP	-	expression tag	UNP Q16851
B	-13	SER	-	expression tag	UNP Q16851
B	-12	HIS	-	expression tag	UNP Q16851
B	-11	PRO	-	expression tag	UNP Q16851
B	-10	GLN	-	expression tag	UNP Q16851
B	-9	PHE	-	expression tag	UNP Q16851
B	-8	GLU	-	expression tag	UNP Q16851
B	-7	LYS	-	expression tag	UNP Q16851
B	-6	GLY	-	expression tag	UNP Q16851
B	-5	ALA	-	expression tag	UNP Q16851
B	-4	LEU	-	expression tag	UNP Q16851
B	-3	VAL	-	expression tag	UNP Q16851
B	-2	PRO	-	expression tag	UNP Q16851
B	-1	ARG	-	expression tag	UNP Q16851
B	0	GLY	-	expression tag	UNP Q16851
B	1	SER	-	expression tag	UNP Q16851
C	-17	MET	-	expression tag	UNP Q16851
C	-16	ALA	-	expression tag	UNP Q16851
C	-15	SER	-	expression tag	UNP Q16851
C	-14	TRP	-	expression tag	UNP Q16851
C	-13	SER	-	expression tag	UNP Q16851
C	-12	HIS	-	expression tag	UNP Q16851
C	-11	PRO	-	expression tag	UNP Q16851
C	-10	GLN	-	expression tag	UNP Q16851
C	-9	PHE	-	expression tag	UNP Q16851
C	-8	GLU	-	expression tag	UNP Q16851
C	-7	LYS	-	expression tag	UNP Q16851
C	-6	GLY	-	expression tag	UNP Q16851
C	-5	ALA	-	expression tag	UNP Q16851
C	-4	LEU	-	expression tag	UNP Q16851
C	-3	VAL	-	expression tag	UNP Q16851
C	-2	PRO	-	expression tag	UNP Q16851
C	-1	ARG	-	expression tag	UNP Q16851
C	0	GLY	-	expression tag	UNP Q16851
C	1	SER	-	expression tag	UNP Q16851
D	-17	MET	-	expression tag	UNP Q16851
D	-16	ALA	-	expression tag	UNP Q16851
D	-15	SER	-	expression tag	UNP Q16851
D	-14	TRP	-	expression tag	UNP Q16851
D	-13	SER	-	expression tag	UNP Q16851
D	-12	HIS	-	expression tag	UNP Q16851

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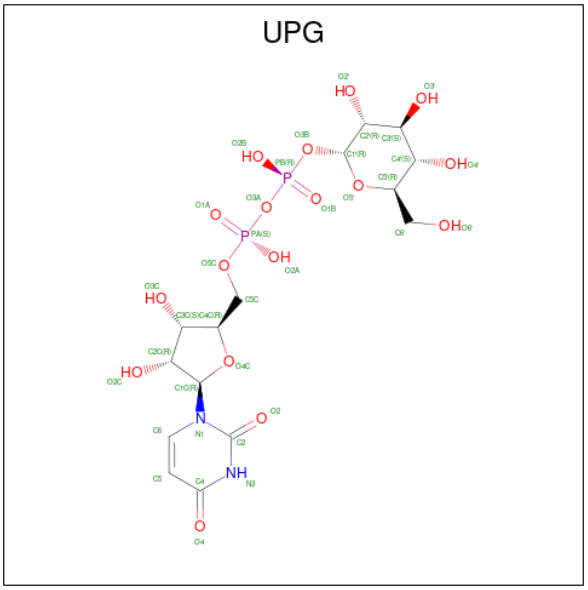
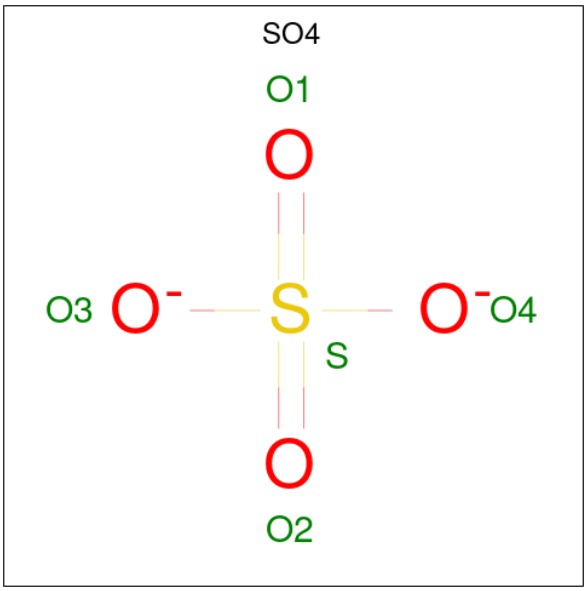
Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	PRO	-	expression tag	UNP Q16851
D	-10	GLN	-	expression tag	UNP Q16851
D	-9	PHE	-	expression tag	UNP Q16851
D	-8	GLU	-	expression tag	UNP Q16851
D	-7	LYS	-	expression tag	UNP Q16851
D	-6	GLY	-	expression tag	UNP Q16851
D	-5	ALA	-	expression tag	UNP Q16851
D	-4	LEU	-	expression tag	UNP Q16851
D	-3	VAL	-	expression tag	UNP Q16851
D	-2	PRO	-	expression tag	UNP Q16851
D	-1	ARG	-	expression tag	UNP Q16851
D	0	GLY	-	expression tag	UNP Q16851
D	1	SER	-	expression tag	UNP Q16851

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	36	15	2	17	2	1	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0

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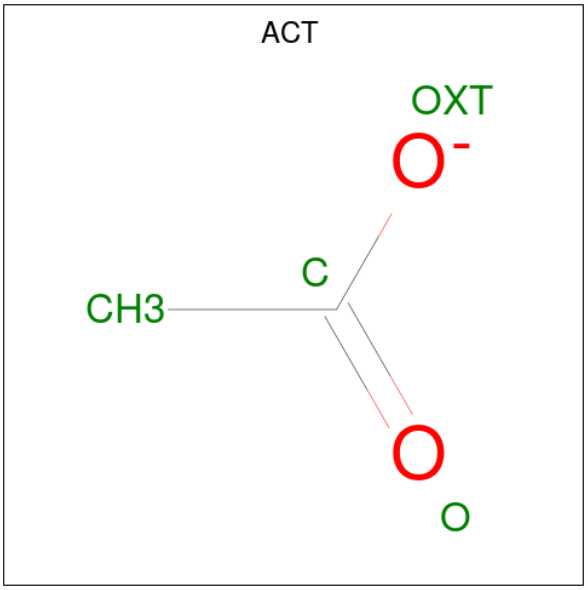
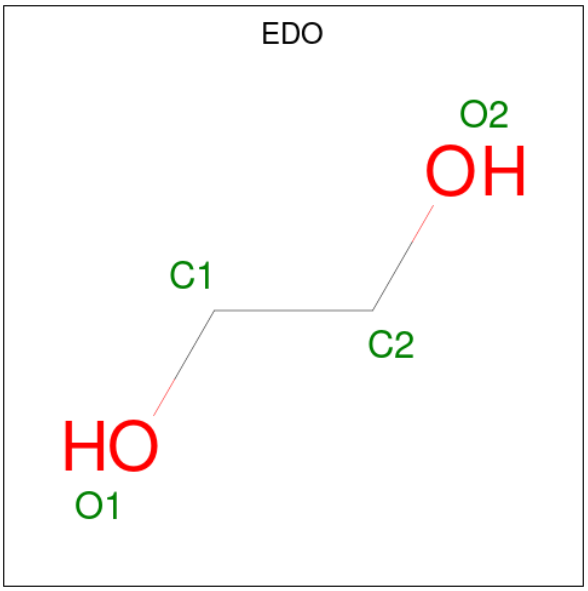
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	D	1	5	4	1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	D	1	4	2	2	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	B	3	3	3	0	0
			Total	Zn		
6	C	4	4	4	0	0
			Total	Zn		
6	D	2	2	2	0	0

- Molecule 7 is water.

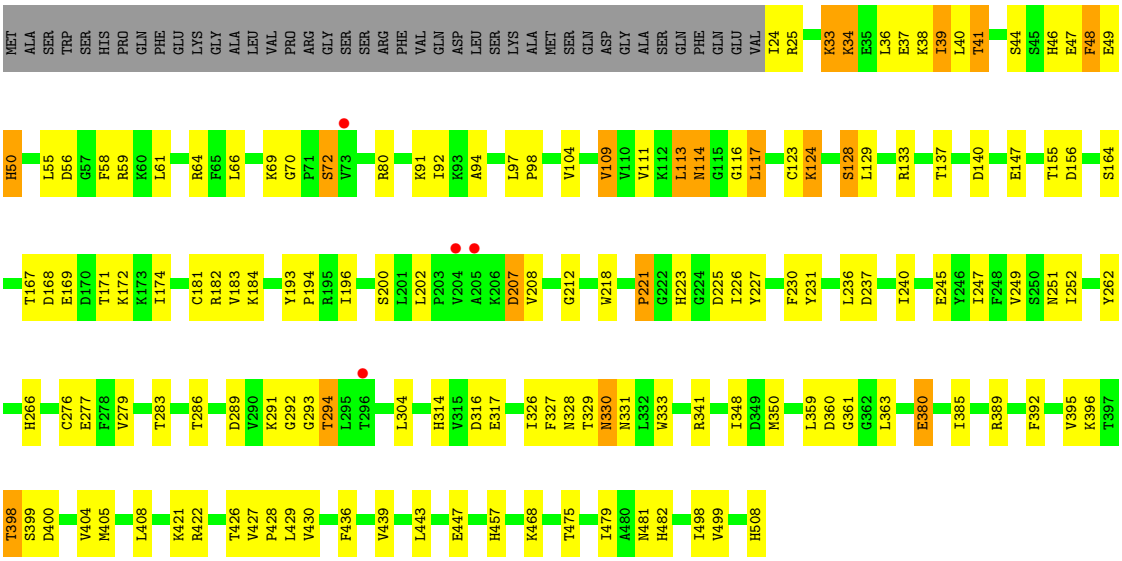
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	34	34	34	0	0
			Total	O		
7	B	25	25	25	0	0
			Total	O		
7	C	26	26	26	0	0
			Total	O		
7	D	32	32	32	0	0

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.

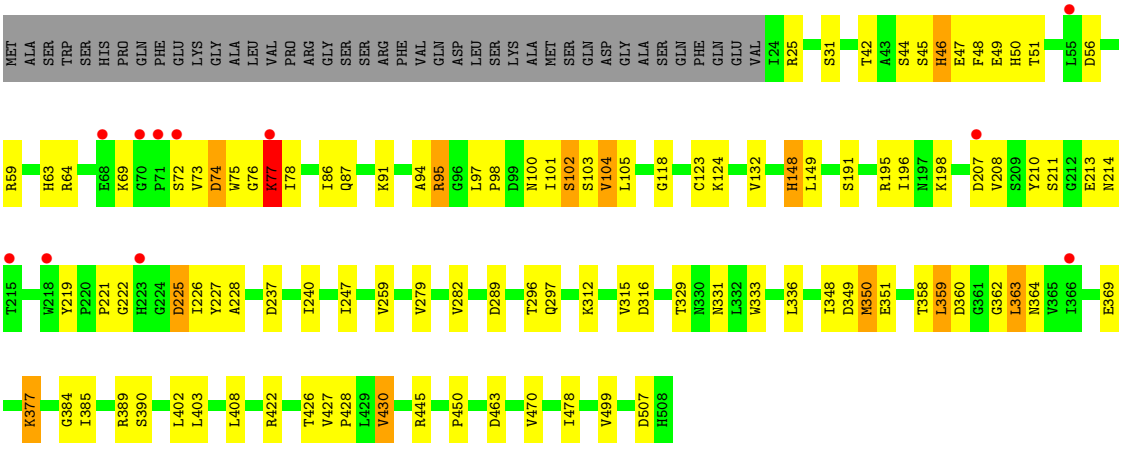
• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain A:



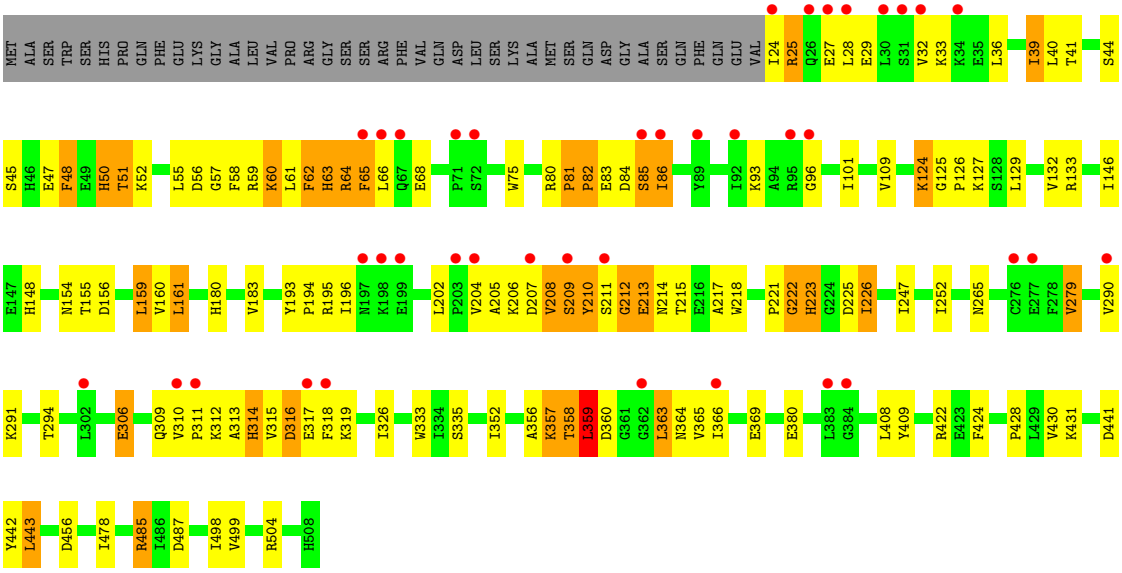
• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain B:



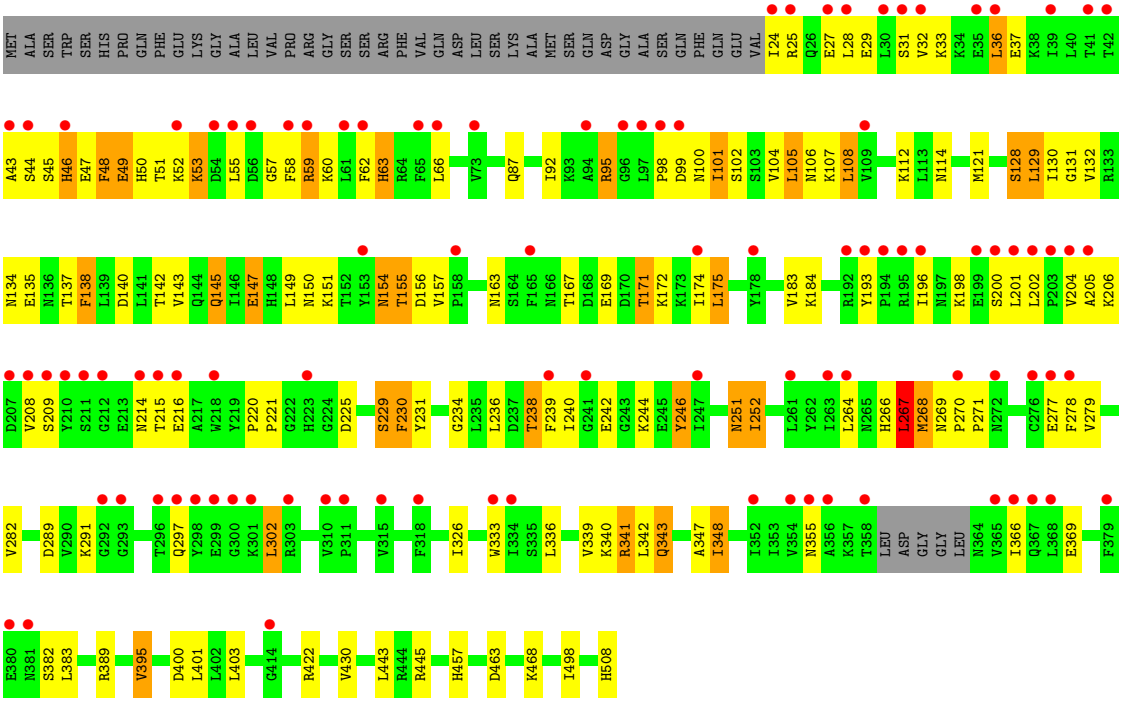
• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain C:



• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.97Å 138.97Å 311.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.62 – 3.35 47.62 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.62-3.35) 100.0 (47.62-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.199 , 0.247 0.203 , 0.250	Depositor DCC
R_{free} test set	2580 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	109.0	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 109.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15591	wwPDB-VP
Average B, all atoms (Å^2)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, SO4, ACT, UPG, EDO

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	0.41	0/3902	0.59	0/5276
1	B	0.38	0/3902	0.54	1/5276 (0.0%)
1	C	0.40	2/3902 (0.1%)	0.58	4/5276 (0.1%)
1	D	0.36	1/3869 (0.0%)	0.55	1/5230 (0.0%)
All	All	0.39	3/15575 (0.0%)	0.57	6/21058 (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	B	0	1
1	C	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	441	ASP	CB-CG	-5.63	1.40	1.51
1	D	147	GLU	CD-OE1	5.23	1.31	1.25
1	C	82	PRO	N-CD	5.20	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	267	LEU	CB-CG-CD2	-8.64	96.32	111.00
1	C	81	PRO	C-N-CD	5.75	140.47	128.40
1	B	222	GLY	N-CA-C	5.53	126.91	113.10
1	C	222	GLY	N-CA-C	5.26	126.25	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	359	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	212	GLY	N-CA-C	-5.10	100.35	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	77	LYS	Peptide
1	C	208	VAL	Peptide
1	C	209	SER	Peptide

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	3831	0	3898	97	0
1	B	3831	0	3898	72	0
1	C	3831	0	3896	116	0
1	D	3799	0	3864	126	0
2	A	36	0	22	5	0
3	A	35	0	0	2	0
3	B	10	0	0	2	0
3	C	15	0	0	1	0
3	D	15	0	0	0	0
4	A	4	0	3	0	0
4	C	4	0	3	0	0
4	D	8	0	6	0	0
5	A	16	0	23	1	0
5	B	20	0	29	0	0
5	C	4	0	5	0	0
5	D	4	0	6	0	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
7	A	34	0	0	4	0
7	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	26	0	0	0	0
7	D	32	0	0	3	0
All	All	15591	0	15653	411	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 13.

All (411) 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:C:208:VAL:O	1:C:212:GLY:N	1.87	1.05
1:C:356:ALA:HB2	1:C:366:ILE:HD13	1.38	1.03
1:C:312:LYS:O	1:C:315:VAL:HG13	1.59	1.02
1:C:222:GLY:C	1:C:223:HIS:HD1	1.62	1.01
1:C:314:HIS:CE1	1:C:317:GLU:OE1	2.15	0.99
1:D:246:TYR:CE2	1:D:267:LEU:HD21	1.99	0.98
1:D:98:PRO:HB2	1:D:101:ILE:CD1	1.94	0.97
1:D:98:PRO:HB2	1:D:101:ILE:HD12	1.44	0.97
1:C:222:GLY:O	1:C:223:HIS:ND1	1.97	0.96
1:A:56:ASP:OD1	1:A:59:ARG:NH1	2.02	0.93
1:A:405:MET:SD	7:A:733:HOH:O	2.29	0.89
1:D:44:SER:HB2	1:D:46:HIS:NE2	1.87	0.88
1:B:77:LYS:CD	1:B:296:THR:HG21	2.04	0.87
1:C:195:ARG:O	1:C:204:VAL:HG13	1.75	0.87
1:C:363:LEU:HD12	1:C:365:VAL:HG22	1.57	0.86
1:C:36:LEU:HA	1:C:39:ILE:HG13	1.56	0.86
1:D:33:LYS:HA	1:D:36:LEU:HD23	1.57	0.85
1:D:43:ALA:HB3	1:D:48:PHE:CE1	2.11	0.85
1:C:195:ARG:C	1:C:204:VAL:HG13	1.98	0.84
1:C:48:PHE:O	1:C:51:THR:OG1	1.95	0.83
1:C:207:ASP:O	1:C:209:SER:HA	1.78	0.83
1:D:205:ALA:O	1:D:214:ASN:ND2	2.13	0.82
1:B:445:ARG:NH2	1:B:463:ASP:OD1	2.15	0.80
1:C:57:GLY:O	1:C:61:LEU:HD23	1.82	0.80
1:C:214:ASN:O	1:C:218:TRP:N	2.13	0.80
1:D:128:SER:O	1:D:137:THR:OG1	2.00	0.79
1:D:151:LYS:NZ	7:D:705:HOH:O	2.15	0.79
1:C:195:ARG:NH1	1:C:215:THR:O	2.17	0.78
1:A:293:GLY:O	1:A:328:ASN:N	2.16	0.78
1:C:312:LYS:O	1:C:315:VAL:CG1	2.31	0.78
1:A:289:ASP:OD2	1:A:389:ARG:NH2	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HD23	1:D:157:VAL:HG22	1.66	0.77
1:D:43:ALA:HB3	1:D:48:PHE:HE1	1.50	0.77
1:C:359:LEU:HD13	1:C:360:ASP:H	1.50	0.76
1:A:123:CYS:SG	7:A:727:HOH:O	2.43	0.76
1:C:213:GLU:OE1	1:C:213:GLU:HA	1.85	0.76
1:C:86:ILE:HD13	1:C:86:ILE:O	1.86	0.75
1:D:105:LEU:HD21	1:D:155:THR:OG1	1.85	0.75
1:C:82:PRO:O	1:C:85:SER:HB3	1.87	0.74
1:D:100:ASN:OD1	1:D:101:ILE:N	2.21	0.74
1:A:168:ASP:OD1	1:A:172:LYS:NZ	2.20	0.73
1:B:349:ASP:OD1	1:B:377:LYS:NZ	2.21	0.73
1:C:159:LEU:HD23	1:C:161:LEU:HD21	1.69	0.73
1:C:214:ASN:OD1	1:C:215:THR:N	2.22	0.73
1:D:48:PHE:O	1:D:51:THR:OG1	2.07	0.72
1:D:102:SER:O	1:D:105:LEU:HD12	1.89	0.72
1:C:314:HIS:HE1	1:C:317:GLU:OE1	1.72	0.72
1:D:47:GLU:O	1:D:50:HIS:NE2	2.22	0.71
1:D:342:LEU:HD13	1:D:347:ALA:HB3	1.70	0.71
1:B:98:PRO:HG2	1:B:101:ILE:HD13	1.72	0.71
1:D:29:GLU:OE2	1:D:63:HIS:ND1	2.24	0.70
1:D:105:LEU:HD23	1:D:157:VAL:CG2	2.20	0.70
1:D:355:ASN:ND2	1:D:369:GLU:OE2	2.25	0.70
1:D:44:SER:HB2	1:D:46:HIS:CE1	2.27	0.69
1:C:24:ILE:HG23	1:C:25:ARG:H	1.57	0.69
1:B:77:LYS:CD	1:B:296:THR:CG2	2.71	0.68
1:D:51:THR:O	1:D:55:LEU:HD12	1.93	0.68
1:B:289:ASP:OD2	1:B:389:ARG:NH2	2.26	0.68
1:C:83:GLU:O	1:C:84:ASP:HB2	1.93	0.68
1:B:47:GLU:HG3	1:B:50:HIS:HB3	1.75	0.67
1:C:64:ARG:NH1	1:C:68:GLU:OE2	2.27	0.67
1:D:47:GLU:HB3	1:D:50:HIS:CD2	2.30	0.67
1:A:293:GLY:O	1:A:327:PHE:HA	1.95	0.67
1:B:101:ILE:O	1:B:104:VAL:N	2.28	0.67
1:C:359:LEU:HD22	1:C:360:ASP:N	2.09	0.67
1:C:363:LEU:HD12	1:C:365:VAL:CG2	2.25	0.67
1:D:231:TYR:HA	1:D:236:LEU:HD23	1.77	0.67
1:D:246:TYR:CD2	1:D:267:LEU:HD21	2.29	0.67
1:C:56:ASP:O	1:C:60:LYS:NZ	2.25	0.67
1:C:86:ILE:HD13	1:C:86:ILE:C	2.15	0.67
1:A:40:LEU:HD11	1:A:48:PHE:CE2	2.31	0.66
1:C:487:ASP:OD2	1:C:504:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:HA	1:A:59:ARG:HD2	1.77	0.66
1:A:133:ARG:NH2	1:A:404:VAL:O	2.29	0.66
1:B:358:THR:OG1	1:B:364:ASN:OD1	2.08	0.66
1:D:47:GLU:HB3	1:D:50:HIS:NE2	2.11	0.65
1:D:98:PRO:HB2	1:D:101:ILE:HD11	1.75	0.65
1:D:105:LEU:HD22	1:D:105:LEU:C	2.17	0.65
1:D:239:PHE:CZ	1:D:336:LEU:HD22	2.32	0.65
1:D:201:LEU:O	1:D:202:LEU:HD12	1.97	0.65
1:A:36:LEU:HA	1:A:39:ILE:HG12	1.79	0.65
1:B:77:LYS:HD3	1:B:296:THR:HG21	1.78	0.65
1:C:146:ILE:CD1	1:C:183:VAL:HG21	2.27	0.65
1:C:294:THR:HG22	1:C:318:PHE:CZ	2.31	0.64
1:C:222:GLY:C	1:C:223:HIS:ND1	2.42	0.64
1:B:77:LYS:HD2	1:B:296:THR:CG2	2.26	0.64
1:C:159:LEU:CD2	1:C:161:LEU:HD21	2.26	0.64
1:B:63:HIS:ND1	3:B:602:SO4:O3	2.31	0.64
1:B:44:SER:O	1:B:45:SER:OG	2.08	0.63
1:C:160:VAL:C	1:C:161:LEU:HD23	2.18	0.63
1:C:363:LEU:HD13	1:C:364:ASN:N	2.12	0.63
1:B:191:SER:CB	1:B:225:ASP:OD2	2.45	0.63
1:B:64:ARG:NH2	1:B:350:MET:O	2.32	0.63
1:A:44:SER:HB2	1:A:46:HIS:ND1	2.12	0.63
1:D:342:LEU:CD1	1:D:347:ALA:HB3	2.28	0.63
1:B:97:LEU:H	1:B:97:LEU:HD23	1.64	0.63
1:D:155:THR:OG1	1:D:156:ASP:N	2.29	0.63
1:D:234:GLY:O	1:D:238:THR:OG1	2.16	0.62
1:D:196:ILE:HD11	1:D:201:LEU:C	2.19	0.62
1:A:70:GLY:O	1:A:72:SER:OG	2.18	0.62
1:A:129:LEU:HD21	1:A:174:ILE:HG12	1.82	0.62
1:D:28:LEU:O	1:D:32:VAL:HG23	1.99	0.62
1:C:310:VAL:N	1:C:311:PRO:HD3	2.15	0.61
1:C:194:PRO:HD3	1:C:218:TRP:HZ3	1.65	0.61
1:C:314:HIS:CE1	1:C:317:GLU:CD	2.73	0.61
1:C:290:VAL:HG22	1:C:319:LYS:HG3	1.81	0.61
1:B:210:TYR:N	1:B:214:ASN:OD1	2.32	0.61
1:B:77:LYS:CG	1:B:296:THR:HG21	2.30	0.61
1:C:363:LEU:HD13	1:C:364:ASN:H	1.64	0.61
1:A:34:LYS:NZ	1:A:37:GLU:OE2	2.29	0.61
1:D:105:LEU:HD22	1:D:106:ASN:N	2.16	0.61
1:C:314:HIS:ND1	1:C:317:GLU:OE1	2.34	0.61
1:D:49:GLU:HG3	1:D:53:LYS:HZ1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:HG3	1:B:47:GLU:O	1.99	0.61
1:C:214:ASN:O	1:C:217:ALA:N	2.32	0.61
1:C:33:LYS:HA	1:C:36:LEU:HD23	1.83	0.60
1:D:240:ILE:HD13	1:D:336:LEU:HD23	1.82	0.60
1:A:293:GLY:HA2	1:A:304:LEU:HD11	1.84	0.60
1:D:196:ILE:HG23	1:D:366:ILE:HG13	1.83	0.60
1:D:302:LEU:HD23	1:D:302:LEU:H	1.67	0.60
1:A:128:SER:O	1:A:137:THR:OG1	2.18	0.60
1:B:191:SER:OG	1:B:225:ASP:OD2	2.17	0.60
1:C:161:LEU:HD23	1:C:161:LEU:N	2.15	0.60
1:D:98:PRO:CB	1:D:101:ILE:HD12	2.24	0.60
1:B:211:SER:H	1:B:214:ASN:HD21	1.49	0.59
1:D:44:SER:CB	1:D:46:HIS:CE1	2.85	0.59
1:A:439:VAL:HG12	1:A:443:LEU:HD13	1.84	0.59
1:A:251:ASN:HD21	2:A:601:UPG:H1'	1.68	0.59
1:A:292:GLY:O	1:A:327:PHE:HB2	2.02	0.59
1:C:146:ILE:HD13	1:C:159:LEU:HD12	1.85	0.59
1:D:236:LEU:HA	1:D:239:PHE:CD2	2.38	0.59
1:B:225:ASP:O	1:B:226:ILE:C	2.40	0.59
1:A:330:ASN:HB2	2:A:601:UPG:H2'	1.86	0.58
1:A:457:HIS:ND1	1:A:475:THR:OG1	2.31	0.58
1:D:163:ASN:ND2	1:D:171:THR:HG21	2.18	0.58
1:A:167:THR:O	1:A:171:THR:OG1	2.10	0.58
1:B:77:LYS:HD2	1:B:296:THR:HG23	1.84	0.58
1:B:296:THR:HG22	1:B:297:GLN:H	1.69	0.58
1:A:44:SER:HB2	1:A:46:HIS:CE1	2.38	0.57
1:B:101:ILE:HG22	1:B:105:LEU:HG	1.85	0.57
1:D:445:ARG:NH2	1:D:463:ASP:OD1	2.36	0.57
1:C:209:SER:OG	1:C:210:TYR:N	2.34	0.57
1:C:210:TYR:N	1:C:210:TYR:CD1	2.72	0.57
1:A:283:THR:HG23	1:A:327:PHE:CE1	2.39	0.57
1:A:396:LYS:HG2	1:A:400:ASP:OD2	2.04	0.57
1:B:149:LEU:HD11	1:B:259:VAL:CG1	2.35	0.57
1:A:39:ILE:HG22	1:A:207:ASP:HA	1.86	0.57
1:B:450:PRO:HB3	1:B:470:VAL:HG13	1.88	0.56
1:D:100:ASN:C	1:D:101:ILE:HG13	2.26	0.56
1:A:293:GLY:O	1:A:327:PHE:CA	2.53	0.56
1:A:147:GLU:OE1	1:A:181:CYS:SG	2.63	0.56
1:B:42:THR:HG21	1:B:207:ASP:CG	2.25	0.56
1:C:214:ASN:HA	1:C:217:ALA:HB3	1.86	0.56
1:D:289:ASP:OD2	1:D:389:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:LEU:HD12	1:D:348:ILE:N	2.20	0.56
1:D:49:GLU:HG3	1:D:53:LYS:NZ	2.21	0.56
1:B:312:LYS:O	1:B:315:VAL:HG12	2.06	0.56
1:D:112:LYS:HD3	1:D:252:ILE:HG23	1.87	0.56
1:D:167:THR:O	1:D:171:THR:OG1	2.23	0.56
1:D:108:LEU:CD1	1:D:264:LEU:HD13	2.36	0.55
1:D:99:ASP:O	1:D:101:ILE:HG13	2.06	0.55
1:D:163:ASN:HD21	1:D:171:THR:HG21	1.71	0.55
1:C:485:ARG:NH2	1:C:487:ASP:OD1	2.39	0.55
1:C:58:PHE:CD2	1:C:194:PRO:HD2	2.40	0.55
1:D:225:ASP:O	1:D:229:SER:OG	2.25	0.55
1:B:87:GLN:OE1	1:B:95:ARG:NH2	2.40	0.55
1:A:482:HIS:NE2	3:A:603:SO4:S	2.78	0.55
1:D:36:LEU:HG	1:D:37:GLU:N	2.21	0.55
1:B:100:ASN:OD1	1:B:103:SER:CB	2.55	0.55
1:C:356:ALA:HB2	1:C:366:ILE:CD1	2.25	0.55
1:A:40:LEU:C	1:A:40:LEU:HD13	2.27	0.54
1:D:108:LEU:HD12	1:D:246:TYR:CE1	2.42	0.54
1:D:230:PHE:HZ	1:D:339:VAL:HG11	1.71	0.54
1:D:106:ASN:OD1	1:D:155:THR:OG1	2.25	0.54
1:A:114:ASN:ND2	1:A:128:SER:OG	2.41	0.53
1:C:159:LEU:HD23	1:C:161:LEU:CD2	2.36	0.53
1:C:32:VAL:HG22	1:C:202:LEU:CD2	2.38	0.53
1:A:40:LEU:HD13	1:A:40:LEU:O	2.07	0.53
1:D:92:ILE:N	1:D:92:ILE:HD12	2.24	0.53
1:D:266:HIS:O	1:D:269:ASN:ND2	2.42	0.53
1:A:34:LYS:NZ	1:A:37:GLU:CD	2.62	0.53
1:C:33:LYS:O	1:C:36:LEU:HG	2.09	0.53
1:C:279:VAL:HG13	1:C:333:TRP:HB2	1.91	0.53
1:D:114:ASN:OD1	1:D:128:SER:OG	2.26	0.52
1:C:65:PHE:HB2	1:C:352:ILE:HG12	1.91	0.52
1:B:225:ASP:O	1:B:227:TYR:N	2.42	0.52
1:B:101:ILE:O	1:B:102:SER:C	2.46	0.52
1:D:266:HIS:CE1	1:D:269:ASN:OD1	2.63	0.52
1:B:296:THR:HG22	1:B:297:GLN:N	2.25	0.52
1:A:109:VAL:HG13	1:A:247:ILE:HG22	1.92	0.52
1:B:101:ILE:HA	1:B:104:VAL:HG23	1.91	0.52
1:B:225:ASP:O	1:B:228:ALA:N	2.43	0.52
1:A:277:GLU:OE2	1:A:380:GLU:N	2.38	0.52
1:C:80:ARG:HB3	1:C:81:PRO:HD2	1.92	0.52
1:C:155:THR:OG1	1:C:156:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASP:HA	1:A:240:ILE:HG22	1.91	0.51
1:C:65:PHE:CE1	1:C:66:LEU:HG	2.45	0.51
1:D:236:LEU:HA	1:D:239:PHE:CE2	2.45	0.51
1:A:329:THR:HG22	1:A:392:PHE:CD1	2.45	0.51
1:A:330:ASN:HB2	2:A:601:UPG:C2'	2.40	0.51
1:C:24:ILE:HG23	1:C:25:ARG:N	2.24	0.51
1:A:279:VAL:HG13	1:A:333:TRP:HB2	1.92	0.51
1:C:146:ILE:HD12	1:C:183:VAL:HG21	1.92	0.51
1:B:45:SER:HA	1:B:48:PHE:HB2	1.93	0.51
1:C:214:ASN:OD1	1:C:215:THR:HG23	2.11	0.51
1:B:351:GLU:N	1:B:351:GLU:OE1	2.43	0.51
1:B:408:LEU:HD21	1:B:428:PRO:CD	2.40	0.51
1:B:191:SER:HB2	1:B:225:ASP:OD2	2.10	0.51
1:C:365:VAL:HG12	1:C:366:ILE:N	2.26	0.51
1:D:92:ILE:HA	1:D:95:ARG:HH12	1.76	0.51
1:C:124:LYS:HG3	1:C:125:GLY:N	2.25	0.51
1:B:221:PRO:HA	1:B:369:GLU:HB3	1.92	0.50
1:D:101:ILE:HG22	1:D:104:VAL:CG1	2.41	0.50
1:B:47:GLU:CG	1:B:50:HIS:HB3	2.42	0.50
1:B:56:ASP:O	1:B:59:ARG:HG2	2.11	0.50
1:B:247:ILE:HG23	1:B:336:LEU:HD21	1.94	0.50
1:C:309:GLN:C	1:C:311:PRO:HD3	2.31	0.50
1:D:267:LEU:HD12	1:D:267:LEU:O	2.10	0.50
1:B:149:LEU:HD11	1:B:259:VAL:HG11	1.94	0.50
1:A:36:LEU:HA	1:A:39:ILE:CG1	2.40	0.50
1:A:314:HIS:NE2	3:A:606:SO4:S	2.85	0.50
1:B:75:TRP:O	1:B:78:ILE:HD13	2.11	0.50
1:C:180:HIS:NE2	3:C:602:SO4:O3	2.45	0.50
1:B:77:LYS:HG3	1:B:296:THR:HG21	1.94	0.50
1:D:100:ASN:CG	1:D:101:ILE:H	2.13	0.50
1:D:143:VAL:O	1:D:147:GLU:N	2.44	0.50
1:D:147:GLU:HG2	1:D:151:LYS:NZ	2.27	0.49
1:B:237:ASP:HA	1:B:240:ILE:HG22	1.93	0.49
1:C:204:VAL:CG2	1:C:205:ALA:N	2.75	0.49
1:C:207:ASP:C	1:C:209:SER:HA	2.33	0.49
1:C:225:ASP:O	1:C:226:ILE:C	2.49	0.49
1:A:97:LEU:HB2	1:A:98:PRO:HD2	1.94	0.49
1:A:277:GLU:OE1	1:A:341:ARG:NH2	2.44	0.49
1:A:117:LEU:HD12	1:A:117:LEU:H	1.77	0.49
1:B:279:VAL:HG13	1:B:333:TRP:HB2	1.94	0.49
1:C:59:ARG:O	1:C:62:PHE:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:HG23	1:C:205:ALA:N	2.26	0.49
1:D:208:VAL:HG21	7:D:731:HOH:O	2.12	0.49
1:C:44:SER:O	1:C:48:PHE:N	2.45	0.49
1:C:204:VAL:CG2	1:C:205:ALA:H	2.26	0.49
1:D:129:LEU:HD21	1:D:174:ILE:HG12	1.93	0.49
1:A:39:ILE:CG2	1:A:207:ASP:HA	2.43	0.48
1:A:124:LYS:HE2	1:A:124:LYS:H	1.78	0.48
1:A:408:LEU:HD21	1:A:428:PRO:CD	2.43	0.48
1:C:357:LYS:HD3	1:C:358:THR:HA	1.95	0.48
1:C:24:ILE:CA	1:C:27:GLU:HG3	2.43	0.48
1:D:131:GLY:HA2	1:D:137:THR:HA	1.95	0.48
1:D:279:VAL:CG1	1:D:333:TRP:HB2	2.43	0.48
1:D:457:HIS:HE1	7:D:707:HOH:O	1.96	0.48
1:A:91:LYS:O	1:A:94:ALA:HB3	2.14	0.48
1:D:105:LEU:HD13	1:D:106:ASN:H	1.77	0.48
1:A:508:HIS:CE1	1:C:431:LYS:HG3	2.49	0.48
1:B:100:ASN:OD1	1:B:103:SER:HB3	2.13	0.48
1:D:130:ILE:HB	1:D:138:PHE:HE1	1.77	0.48
1:B:329:THR:HG23	1:B:331:ASN:H	1.77	0.48
1:D:24:ILE:N	1:D:27:GLU:OE1	2.47	0.47
1:D:137:THR:O	1:D:140:ASP:N	2.47	0.47
1:B:359:LEU:O	1:B:362:GLY:N	2.47	0.47
1:D:107:LYS:HE3	1:D:246:TYR:OH	2.13	0.47
1:D:172:LYS:HA	1:D:175:LEU:HD23	1.97	0.47
1:B:73:VAL:HG22	1:B:74:ASP:O	2.14	0.47
1:A:124:LYS:CE	7:A:727:HOH:O	2.61	0.47
1:D:59:ARG:HG3	1:D:60:LYS:N	2.29	0.47
1:D:167:THR:O	1:D:171:THR:N	2.43	0.47
1:A:283:THR:HG23	1:A:327:PHE:HE1	1.80	0.47
1:B:42:THR:CG2	1:B:207:ASP:OD2	2.63	0.47
1:C:208:VAL:O	1:C:211:SER:OG	2.28	0.47
1:D:62:PHE:CE1	1:D:66:LEU:HD12	2.50	0.47
1:D:108:LEU:HA	1:D:246:TYR:CD1	2.50	0.47
1:A:231:TYR:HA	1:A:236:LEU:HD22	1.97	0.47
1:A:316:ASP:OD1	1:A:317:GLU:N	2.47	0.47
1:B:207:ASP:OD1	1:B:208:VAL:N	2.47	0.47
1:D:340:LYS:HG3	1:D:341:ARG:N	2.28	0.47
1:C:50:HIS:ND1	1:C:50:HIS:C	2.68	0.47
1:D:201:LEU:C	1:D:202:LEU:HD12	2.34	0.47
1:A:40:LEU:HD11	1:A:48:PHE:HE2	1.75	0.46
1:C:313:ALA:O	1:C:314:HIS:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ASN:O	1:D:101:ILE:HG13	2.15	0.46
1:A:34:LYS:HZ2	1:A:37:GLU:CD	2.18	0.46
1:D:236:LEU:HD12	1:D:236:LEU:C	2.36	0.46
1:C:208:VAL:C	1:C:211:SER:HG	2.15	0.46
1:A:137:THR:HG23	1:A:140:ASP:H	1.81	0.46
1:B:148:HIS:ND1	3:B:601:SO4:O4	2.40	0.46
1:A:479:ILE:HG23	1:A:479:ILE:O	2.16	0.46
1:D:183:VAL:HG22	1:D:184:LYS:N	2.30	0.46
1:A:50:HIS:ND1	1:A:50:HIS:C	2.70	0.46
1:A:207:ASP:N	1:A:207:ASP:OD1	2.49	0.46
1:D:239:PHE:CE2	1:D:336:LEU:HD22	2.50	0.46
1:A:58:PHE:CD2	1:A:194:PRO:HD2	2.51	0.45
1:B:91:LYS:O	1:B:94:ALA:HB3	2.16	0.45
1:B:86:ILE:HA	1:B:384:GLY:O	2.16	0.45
1:A:58:PHE:CD1	1:A:58:PHE:C	2.90	0.45
1:C:32:VAL:HG22	1:C:202:LEU:HD22	1.96	0.45
1:A:61:LEU:HD12	1:A:193:TYR:HE2	1.80	0.45
1:C:146:ILE:HD11	1:C:183:VAL:HG21	1.97	0.45
1:D:268:MET:HB2	1:D:270:PRO:HD3	1.98	0.45
1:C:50:HIS:ND1	1:C:51:THR:N	2.65	0.45
1:D:279:VAL:HA	1:D:383:LEU:O	2.17	0.45
1:A:58:PHE:HD2	1:A:193:TYR:HB3	1.81	0.45
1:A:113:LEU:HD23	1:A:113:LEU:N	2.31	0.45
1:B:359:LEU:CD1	1:B:360:ASP:H	2.29	0.45
1:A:236:LEU:HD23	1:A:237:ASP:N	2.32	0.45
1:B:408:LEU:HD21	1:B:428:PRO:CG	2.46	0.45
1:A:36:LEU:HD13	1:A:55:LEU:HG	1.99	0.45
1:C:44:SER:OG	1:C:47:GLU:HB2	2.17	0.45
1:D:209:SER:O	1:D:214:ASN:HB2	2.17	0.45
1:C:193:TYR:CD2	1:C:221:PRO:HG3	2.52	0.45
1:D:108:LEU:HA	1:D:246:TYR:HD1	1.82	0.45
1:A:155:THR:OG1	1:A:156:ASP:N	2.50	0.44
1:A:33:LYS:HD3	1:A:34:LYS:HD2	1.99	0.44
1:C:133:ARG:NH1	1:C:409:TYR:O	2.50	0.44
1:C:194:PRO:HD3	1:C:218:TRP:CZ3	2.48	0.44
1:D:302:LEU:HD21	1:D:382:SER:OG	2.17	0.44
1:A:286:THR:N	1:A:289:ASP:OD1	2.42	0.44
1:A:508:HIS:O	1:A:508:HIS:ND1	2.51	0.44
1:C:36:LEU:HD12	1:C:36:LEU:C	2.37	0.44
1:C:146:ILE:HD13	1:C:159:LEU:CD1	2.48	0.44
1:A:294:THR:OG1	1:A:326:ILE:O	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:HD13	1:B:360:ASP:H	1.83	0.44
1:C:222:GLY:H	1:C:369:GLU:HB2	1.83	0.44
1:C:315:VAL:HG23	1:C:316:ASP:N	2.32	0.44
1:A:38:LYS:O	1:A:41:THR:HG22	2.17	0.44
1:D:44:SER:OG	1:D:46:HIS:CE1	2.70	0.44
1:D:231:TYR:CD2	1:D:343:GLN:NE2	2.86	0.44
1:D:242:GLU:HG2	1:D:244:LYS:HE3	2.00	0.44
1:A:48:PHE:CD1	1:A:49:GLU:N	2.85	0.44
1:A:194:PRO:HD3	1:A:218:TRP:HZ3	1.81	0.44
1:B:195:ARG:HE	1:B:219:TYR:HB3	1.83	0.44
1:A:58:PHE:CD2	1:A:193:TYR:HB3	2.52	0.43
1:B:76:GLY:C	1:B:78:ILE:HA	2.38	0.43
1:C:58:PHE:O	1:C:61:LEU:HB2	2.17	0.43
1:D:134:ASN:C	1:D:135:GLU:HG3	2.37	0.43
2:A:601:UPG:C6	2:A:601:UPG:H5C1	2.48	0.43
1:C:40:LEU:HD23	1:C:40:LEU:C	2.38	0.43
1:C:32:VAL:HG22	1:C:202:LEU:HD23	2.00	0.43
1:D:108:LEU:HD13	1:D:264:LEU:HD13	2.00	0.43
1:C:211:SER:HG	1:C:212:GLY:H	1.66	0.43
1:D:87:GLN:HE22	1:D:266:HIS:CE1	2.37	0.43
1:C:314:HIS:ND1	1:C:317:GLU:CD	2.71	0.43
1:D:236:LEU:HA	1:D:239:PHE:HD2	1.83	0.43
1:A:124:LYS:HE3	7:A:727:HOH:O	2.18	0.43
1:C:24:ILE:N	1:C:27:GLU:HG3	2.33	0.43
1:C:408:LEU:HD21	1:C:428:PRO:CD	2.48	0.43
1:D:57:GLY:HA2	1:D:60:LYS:HG2	2.01	0.43
1:D:403:LEU:HG	1:D:430:VAL:HG11	2.01	0.43
1:A:200:SER:HB2	1:A:202:LEU:HD23	1.99	0.43
1:C:357:LYS:HZ2	1:C:359:LEU:HB3	1.84	0.43
1:D:29:GLU:OE2	1:D:63:HIS:CE1	2.72	0.43
1:D:51:THR:C	1:D:55:LEU:HD12	2.39	0.43
1:D:108:LEU:CD1	1:D:264:LEU:CD1	2.97	0.43
1:D:92:ILE:HA	1:D:95:ARG:NH1	2.34	0.43
1:D:150:ASN:O	1:D:154:ASN:N	2.52	0.43
1:B:101:ILE:O	1:B:104:VAL:HG23	2.19	0.42
1:B:358:THR:HA	1:B:363:LEU:O	2.19	0.42
1:D:251:ASN:OD1	1:D:251:ASN:N	2.52	0.42
1:D:270:PRO:N	1:D:271:PRO:HD2	2.33	0.42
1:A:266:HIS:NE2	5:A:612:EDO:O1	2.49	0.42
1:A:360:ASP:OD1	1:A:361:GLY:N	2.53	0.42
1:C:159:LEU:CD2	1:C:161:LEU:CD2	2.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ASN:C	1:C:217:ALA:H	2.19	0.42
1:A:396:LYS:NZ	1:A:400:ASP:OD1	2.52	0.42
1:B:359:LEU:HD13	1:B:360:ASP:N	2.33	0.42
1:C:478:ILE:HG12	1:C:499:VAL:CG1	2.49	0.42
1:A:36:LEU:CA	1:A:39:ILE:HG12	2.47	0.42
1:A:208:VAL:HG11	1:A:212:GLY:HA3	2.02	0.42
1:A:395:VAL:HG13	1:A:400:ASP:HB2	2.01	0.42
1:B:478:ILE:HG12	1:B:499:VAL:CG1	2.49	0.42
1:C:357:LYS:HD3	1:C:358:THR:CA	2.50	0.42
1:A:227:TYR:CD2	1:A:348:ILE:CD1	3.03	0.42
1:B:403:LEU:HG	1:B:430:VAL:HG11	2.02	0.42
1:C:40:LEU:HD23	1:C:40:LEU:O	2.19	0.42
1:D:215:THR:HG23	1:D:216:GLU:N	2.35	0.42
1:A:447:GLU:HG2	1:A:468:LYS:HG3	2.02	0.42
1:B:118:GLY:O	1:B:123:CYS:N	2.51	0.42
1:C:29:GLU:OE1	1:C:63:HIS:ND1	2.52	0.42
1:A:183:VAL:HG22	1:A:184:LYS:N	2.35	0.42
1:D:105:LEU:HD13	1:D:106:ASN:N	2.34	0.42
1:D:57:GLY:O	1:D:60:LYS:HG2	2.20	0.41
1:D:142:THR:HA	1:D:145:GLN:HG3	2.02	0.41
1:A:226:ILE:O	1:A:230:PHE:HB2	2.20	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.89	0.41
1:D:508:HIS:O	1:D:508:HIS:ND1	2.53	0.41
1:A:329:THR:O	1:A:331:ASN:N	2.43	0.41
1:A:92:ILE:HG22	1:A:262:TYR:HB3	2.02	0.41
1:B:44:SER:OG	1:B:46:HIS:N	2.54	0.41
1:B:100:ASN:OD1	1:B:103:SER:HB2	2.20	0.41
1:C:442:TYR:CD2	1:C:443:LEU:HD13	2.56	0.41
1:A:193:TYR:CG	1:A:221:PRO:HG3	2.56	0.41
1:C:55:LEU:O	1:C:58:PHE:HB3	2.20	0.41
1:D:121:MET:HE1	1:D:401:LEU:HD11	2.02	0.41
1:A:395:VAL:O	1:A:395:VAL:HG12	2.20	0.41
1:D:47:GLU:O	1:D:50:HIS:CD2	2.74	0.41
1:A:111:VAL:HB	1:A:249:VAL:HG12	2.02	0.41
1:A:164:SER:O	1:A:168:ASP:N	2.52	0.41
1:C:28:LEU:O	1:C:32:VAL:HG23	2.21	0.41
1:C:58:PHE:CE2	1:C:194:PRO:HG2	2.56	0.41
1:C:62:PHE:CE1	1:C:65:PHE:CE1	3.08	0.41
1:D:55:LEU:HD12	1:D:55:LEU:H	1.86	0.41
1:D:107:LYS:O	1:D:244:LYS:HB3	2.20	0.41
1:D:220:PRO:HA	1:D:221:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:THR:HG21	1:A:436:PHE:O	2.20	0.41
1:B:315:VAL:HG13	1:B:316:ASP:N	2.35	0.41
1:D:100:ASN:CG	1:D:101:ILE:N	2.73	0.41
1:A:171:THR:O	1:A:174:ILE:HG13	2.21	0.40
1:C:96:GLY:O	1:C:265:ASN:ND2	2.45	0.40
1:C:306:GLU:O	1:C:310:VAL:HG23	2.20	0.40
1:C:126:PRO:HD2	1:C:129:LEU:HD22	2.03	0.40
1:D:395:VAL:HG23	1:D:400:ASP:HB2	2.04	0.40
1:A:116:GLY:N	2:A:601:UPG:H2C	2.37	0.40
1:D:167:THR:C	1:D:171:THR:HG1	2.21	0.40
1:D:58:PHE:CD2	1:D:193:TYR:HB3	2.56	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	483/526 (92%)	460 (95%)	22 (5%)	1 (0%)	47 78
1	B	483/526 (92%)	463 (96%)	20 (4%)	0	100 100
1	C	483/526 (92%)	467 (97%)	16 (3%)	0	100 100
1	D	476/526 (90%)	454 (95%)	21 (4%)	1 (0%)	47 78
All	All	1925/2104 (92%)	1844 (96%)	79 (4%)	2 (0%)	51 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	101	ILE
1	A	221	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	433/467 (93%)	384 (89%)	49 (11%)	6 23
1	B	433/467 (93%)	400 (92%)	33 (8%)	13 41
1	C	433/467 (93%)	380 (88%)	53 (12%)	5 19
1	D	430/467 (92%)	378 (88%)	52 (12%)	5 20
All	All	1729/1868 (93%)	1542 (89%)	187 (11%)	6 25

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	25	ARG
1	A	33	LYS
1	A	34	LYS
1	A	39	ILE
1	A	41	THR
1	A	47	GLU
1	A	48	PHE
1	A	50	HIS
1	A	64	ARG
1	A	66	LEU
1	A	69	LYS
1	A	72	SER
1	A	80	ARG
1	A	104	VAL
1	A	109	VAL
1	A	113	LEU
1	A	114	ASN
1	A	117	LEU
1	A	124	LYS
1	A	128	SER
1	A	169	GLU
1	A	182	ARG
1	A	196	ILE

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Mol	Chain	Res	Type
1	A	207	ASP
1	A	223	HIS
1	A	225	ASP
1	A	245	GLU
1	A	252	ILE
1	A	276	CYS
1	A	291	LYS
1	A	294	THR
1	A	330	ASN
1	A	350	MET
1	A	359	LEU
1	A	363	LEU
1	A	380	GLU
1	A	385	ILE
1	A	398	THR
1	A	399	SER
1	A	421	LYS
1	A	422	ARG
1	A	426	THR
1	A	427	VAL
1	A	429	LEU
1	A	430	VAL
1	A	481	ASN
1	A	498	ILE
1	A	499	VAL
1	B	25	ARG
1	B	31	SER
1	B	46	HIS
1	B	49	GLU
1	B	51	THR
1	B	69	LYS
1	B	72	SER
1	B	74	ASP
1	B	77	LYS
1	B	95	ARG
1	B	102	SER
1	B	104	VAL
1	B	124	LYS
1	B	132	VAL
1	B	148	HIS
1	B	196	ILE
1	B	198	LYS

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Mol	Chain	Res	Type
1	B	213	GLU
1	B	225	ASP
1	B	282	VAL
1	B	348	ILE
1	B	350	MET
1	B	359	LEU
1	B	363	LEU
1	B	377	LYS
1	B	385	ILE
1	B	390	SER
1	B	402	LEU
1	B	422	ARG
1	B	426	THR
1	B	427	VAL
1	B	430	VAL
1	B	507	ASP
1	C	25	ARG
1	C	39	ILE
1	C	41	THR
1	C	45	SER
1	C	48	PHE
1	C	50	HIS
1	C	51	THR
1	C	52	LYS
1	C	60	LYS
1	C	62	PHE
1	C	63	HIS
1	C	64	ARG
1	C	65	PHE
1	C	75	TRP
1	C	85	SER
1	C	86	ILE
1	C	93	LYS
1	C	101	ILE
1	C	109	VAL
1	C	124	LYS
1	C	127	LYS
1	C	132	VAL
1	C	148	HIS
1	C	154	ASN
1	C	159	LEU
1	C	161	LEU

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Mol	Chain	Res	Type
1	C	196	ILE
1	C	206	LYS
1	C	210	TYR
1	C	213	GLU
1	C	223	HIS
1	C	226	ILE
1	C	247	ILE
1	C	252	ILE
1	C	279	VAL
1	C	291	LYS
1	C	306	GLU
1	C	314	HIS
1	C	316	ASP
1	C	326	ILE
1	C	335	SER
1	C	357	LYS
1	C	358	THR
1	C	359	LEU
1	C	363	LEU
1	C	380	GLU
1	C	422	ARG
1	C	424	PHE
1	C	430	VAL
1	C	443	LEU
1	C	456	ASP
1	C	485	ARG
1	C	498	ILE
1	D	25	ARG
1	D	31	SER
1	D	36	LEU
1	D	45	SER
1	D	46	HIS
1	D	48	PHE
1	D	49	GLU
1	D	52	LYS
1	D	53	LYS
1	D	59	ARG
1	D	63	HIS
1	D	95	ARG
1	D	105	LEU
1	D	108	LEU
1	D	128	SER

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Mol	Chain	Res	Type
1	D	129	LEU
1	D	132	VAL
1	D	138	PHE
1	D	145	GLN
1	D	149	LEU
1	D	154	ASN
1	D	155	THR
1	D	169	GLU
1	D	171	THR
1	D	175	LEU
1	D	198	LYS
1	D	200	SER
1	D	204	VAL
1	D	206	LYS
1	D	229	SER
1	D	230	PHE
1	D	238	THR
1	D	246	TYR
1	D	251	ASN
1	D	252	ILE
1	D	267	LEU
1	D	268	MET
1	D	277	GLU
1	D	278	PHE
1	D	282	VAL
1	D	291	LYS
1	D	297	GLN
1	D	302	LEU
1	D	326	ILE
1	D	341	ARG
1	D	343	GLN
1	D	348	ILE
1	D	395	VAL
1	D	422	ARG
1	D	443	LEU
1	D	468	LYS
1	D	498	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN

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Mol	Chain	Res	Type
1	A	251	ASN
1	C	314	HIS
1	D	87	GLN
1	D	266	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 11 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
4	ACT	D	604	-	3,3,3	0.73	0	3,3,3	1.32	0
3	SO4	D	603	-	4,4,4	0.16	0	6,6,6	0.04	0
5	EDO	A	610	-	3,3,3	0.53	0	2,2,2	0.03	0
5	EDO	A	612	-	3,3,3	0.55	0	2,2,2	0.02	0
5	EDO	B	604	-	3,3,3	0.50	0	2,2,2	0.32	0
5	EDO	B	603	-	3,3,3	0.51	0	2,2,2	0.11	0
3	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.15	0
5	EDO	B	605	-	3,3,3	0.36	0	2,2,2	0.07	0
3	SO4	A	607	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	A	603	-	4,4,4	0.18	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	604	-	4,4,4	0.28	0	6,6,6	0.52	0
4	ACT	A	609	-	3,3,3	0.75	0	3,3,3	1.43	0
5	EDO	A	613	-	3,3,3	1.40	0	2,2,2	0.33	0
4	ACT	C	604	-	3,3,3	0.74	0	3,3,3	1.33	0
3	SO4	B	601	-	4,4,4	0.30	0	6,6,6	0.31	0
2	UPG	A	601	-	35,38,38	2.04	8 (22%)	53,58,58	1.51	8 (15%)
3	SO4	D	601	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	C	603	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	B	602	-	4,4,4	0.12	0	6,6,6	0.16	0
5	EDO	A	611	-	3,3,3	0.52	0	2,2,2	0.12	0
5	EDO	B	606	-	3,3,3	0.49	0	2,2,2	0.28	0
3	SO4	A	608	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	C	602	-	4,4,4	0.21	0	6,6,6	0.22	0
5	EDO	B	607	-	3,3,3	0.51	0	2,2,2	0.04	0
5	EDO	D	606	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	C	605	-	3,3,3	0.60	0	2,2,2	0.24	0
3	SO4	C	601	-	4,4,4	0.21	0	6,6,6	0.20	0
3	SO4	A	606	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	D	602	-	4,4,4	0.11	0	6,6,6	0.16	0
3	SO4	A	602	-	4,4,4	0.11	0	6,6,6	0.36	0
4	ACT	D	605	-	3,3,3	0.78	0	3,3,3	1.39	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
5	EDO	B	607	-	-	1/1/1/1	-
5	EDO	D	606	-	-	1/1/1/1	-
5	EDO	A	610	-	-	1/1/1/1	-
5	EDO	A	612	-	-	1/1/1/1	-
5	EDO	B	604	-	-	0/1/1/1	-
5	EDO	A	613	-	-	0/1/1/1	-
5	EDO	B	603	-	-	1/1/1/1	-
5	EDO	C	605	-	-	1/1/1/1	-
5	EDO	A	611	-	-	1/1/1/1	-
5	EDO	B	606	-	-	1/1/1/1	-
2	UPG	A	601	-	-	12/23/59/59	0/3/3/3
5	EDO	B	605	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	UPG	PB-O3B	8.43	1.82	1.60
2	A	601	UPG	PA-O5C	3.48	1.73	1.59
2	A	601	UPG	C2-N1	3.28	1.43	1.38
2	A	601	UPG	O5C-C5C	-2.75	1.34	1.44
2	A	601	UPG	C1C-N1	2.34	1.54	1.47
2	A	601	UPG	C4'-C5'	2.22	1.57	1.53
2	A	601	UPG	C4-N3	2.21	1.42	1.38
2	A	601	UPG	C3C-C2C	2.01	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	UPG	O5'-C1'-O3B	4.76	117.59	111.36
2	A	601	UPG	O3B-PB-O1B	-3.31	97.05	109.47
2	A	601	UPG	C4-N3-C2	-2.48	123.31	126.58
2	A	601	UPG	C3'-C4'-C5'	-2.42	105.92	110.24
2	A	601	UPG	C1'-O5'-C5'	2.36	118.32	113.69
2	A	601	UPG	O3A-PB-O3B	2.17	106.86	102.48
2	A	601	UPG	C6'-C5'-C4'	-2.15	107.98	113.00
2	A	601	UPG	N3-C2-N1	2.06	117.63	114.89

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	UPG	C3C-C4C-C5C-O5C
2	A	601	UPG	C5C-O5C-PA-O2A
2	A	601	UPG	C5C-O5C-PA-O3A
2	A	601	UPG	O5'-C1'-O3B-PB
2	A	601	UPG	O4C-C4C-C5C-O5C
5	A	610	EDO	O1-C1-C2-O2
5	B	603	EDO	O1-C1-C2-O2
5	C	605	EDO	O1-C1-C2-O2
5	D	606	EDO	O1-C1-C2-O2
2	A	601	UPG	O5'-C5'-C6'-O6'
5	A	612	EDO	O1-C1-C2-O2
5	B	606	EDO	O1-C1-C2-O2
2	A	601	UPG	C1'-O3B-PB-O3A
2	A	601	UPG	PB-O3A-PA-O5C
2	A	601	UPG	C4C-C5C-O5C-PA
5	B	607	EDO	O1-C1-C2-O2
5	A	611	EDO	O1-C1-C2-O2

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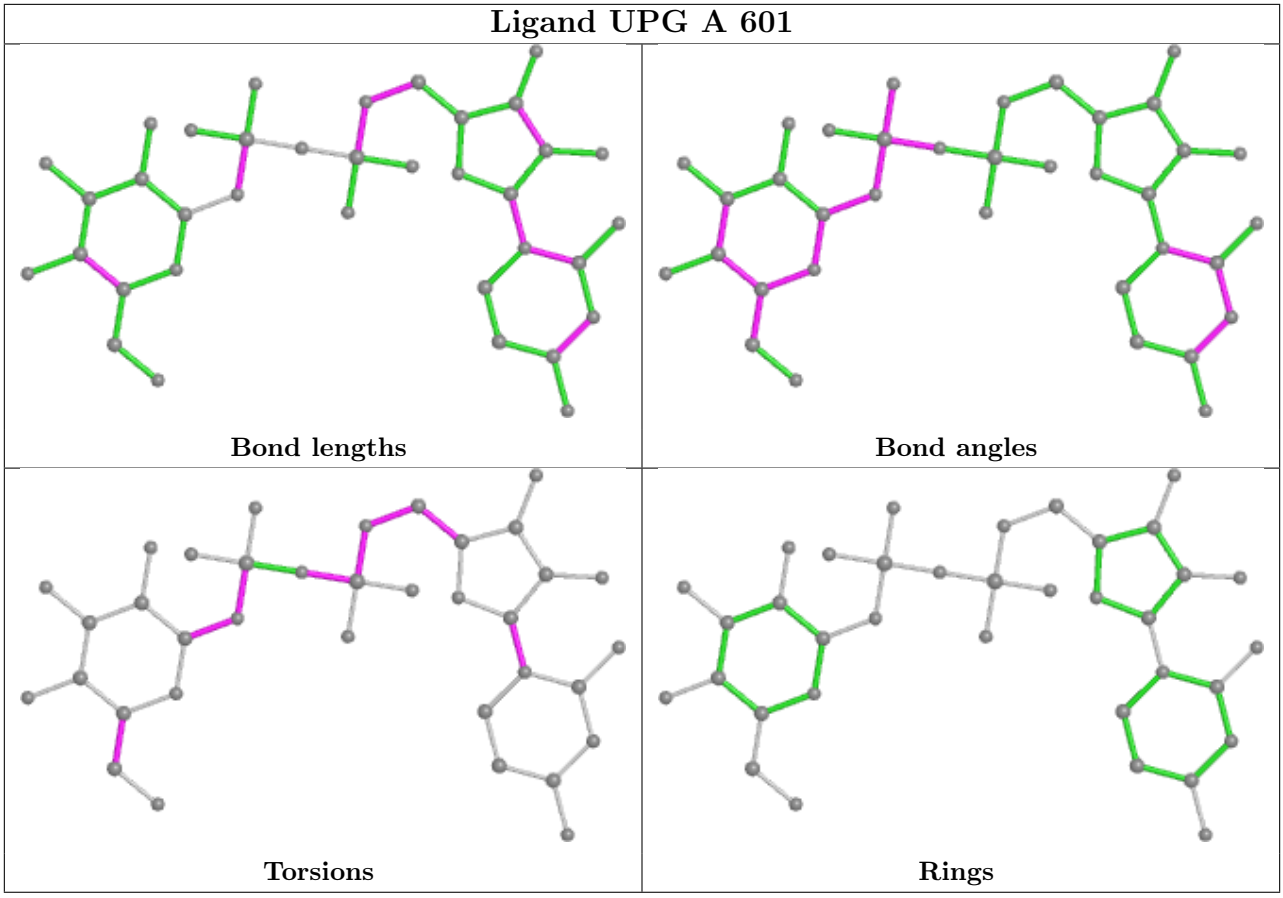
Mol	Chain	Res	Type	Atoms
2	A	601	UPG	O4C-C1C-N1-C6
2	A	601	UPG	C5C-O5C-PA-O1A
2	A	601	UPG	C2C-C1C-N1-C6

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	612	EDO	1	0
3	A	603	SO4	1	0
3	B	601	SO4	1	0
2	A	601	UPG	5	0
3	B	602	SO4	1	0
3	C	602	SO4	1	0
3	A	606	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	485/526 (92%)	-0.07	4 (0%) 86 89	67, 112, 200, 282	0
1	B	485/526 (92%)	-0.02	11 (2%) 60 63	76, 119, 220, 340	0
1	C	485/526 (92%)	0.33	39 (8%) 12 14	70, 148, 274, 437	0
1	D	480/526 (91%)	0.83	99 (20%) 1 1	67, 209, 313, 389	0
All	All	1935/2104 (91%)	0.27	153 (7%) 12 14	67, 134, 282, 437	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	65	PHE	8.0
1	D	56	ASP	7.9
1	B	71	PRO	7.2
1	C	384	GLY	6.7
1	C	383	LEU	6.7
1	D	54	ASP	6.5
1	D	43	ALA	6.2
1	D	55	LEU	6.0
1	D	277	GLU	6.0
1	D	202	LEU	5.9
1	C	85	SER	5.3
1	D	42	THR	5.2
1	D	366	ILE	5.2
1	D	352	ILE	5.1
1	D	209	SER	5.1
1	D	367	GLN	4.9
1	D	203	PRO	4.8
1	D	41	THR	4.8
1	D	310	VAL	4.8
1	D	24	ILE	4.7
1	C	28	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	296	THR	4.6
1	D	207	ASP	4.6
1	D	36	LEU	4.6
1	A	205	ALA	4.5
1	B	72	SER	4.5
1	D	58	PHE	4.4
1	D	193	TYR	4.4
1	D	44	SER	4.3
1	D	31	SER	4.3
1	C	30	LEU	4.3
1	D	96	GLY	4.2
1	D	61	LEU	4.1
1	D	208	VAL	4.0
1	D	210	TYR	4.0
1	C	203	PRO	4.0
1	D	365	VAL	4.0
1	C	96	GLY	3.9
1	D	39	ILE	3.9
1	D	381	ASN	3.9
1	D	241	GLY	3.9
1	D	356	ALA	3.9
1	B	207	ASP	3.9
1	D	354	VAL	3.8
1	D	25	ARG	3.8
1	C	34	LYS	3.8
1	D	62	PHE	3.8
1	C	95	ARG	3.8
1	D	379	PHE	3.8
1	D	300	GLY	3.7
1	D	59	ARG	3.7
1	C	277	GLU	3.7
1	D	27	GLU	3.7
1	B	77	LYS	3.6
1	D	46	HIS	3.6
1	D	380	GLU	3.6
1	D	297	GLN	3.6
1	D	211	SER	3.5
1	D	194	PRO	3.5
1	C	27	GLU	3.5
1	D	368	LEU	3.4
1	C	71	PRO	3.4
1	D	97	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	201	LEU	3.3
1	D	299	GLU	3.3
1	C	92	ILE	3.3
1	D	28	LEU	3.3
1	D	239	PHE	3.3
1	D	272	ASN	3.2
1	D	298	TYR	3.2
1	D	204	VAL	3.2
1	B	218	TRP	3.2
1	D	94	ALA	3.2
1	D	355	ASN	3.1
1	A	204	VAL	3.1
1	C	65	PHE	3.1
1	D	334	ILE	3.0
1	D	303	ARG	3.0
1	C	199	GLU	3.0
1	D	73	VAL	2.9
1	D	301	LYS	2.9
1	D	32	VAL	2.9
1	C	318	PHE	2.9
1	D	196	ILE	2.9
1	B	366	ILE	2.9
1	D	270	PRO	2.9
1	D	311	PRO	2.9
1	B	55	LEU	2.9
1	C	362	GLY	2.9
1	D	52	LYS	2.9
1	C	209	SER	2.8
1	D	278	PHE	2.8
1	D	200	SER	2.8
1	C	204	VAL	2.8
1	C	31	SER	2.8
1	D	247	ILE	2.8
1	C	66	LEU	2.8
1	D	98	PRO	2.7
1	D	292	GLY	2.7
1	D	223	HIS	2.7
1	A	296	THR	2.7
1	D	30	LEU	2.7
1	D	192	ARG	2.7
1	D	261	LEU	2.7
1	D	276	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	223	HIS	2.7
1	D	165	PHE	2.7
1	D	174	ILE	2.7
1	C	317	GLU	2.6
1	D	315	VAL	2.6
1	D	178	TYR	2.6
1	D	218	TRP	2.6
1	C	211	SER	2.5
1	D	214	ASN	2.5
1	D	99	ASP	2.5
1	D	153	TYR	2.5
1	C	207	ASP	2.5
1	C	72	SER	2.5
1	C	26	GLN	2.5
1	C	32	VAL	2.4
1	C	276	CYS	2.4
1	C	366	ILE	2.4
1	D	318	PHE	2.4
1	C	198	LYS	2.4
1	C	67	GLN	2.4
1	C	24	ILE	2.4
1	C	310	VAL	2.4
1	D	66	LEU	2.3
1	D	358	THR	2.3
1	D	35	GLU	2.2
1	B	68	GLU	2.2
1	D	414	GLY	2.2
1	B	215	THR	2.2
1	A	73	VAL	2.2
1	B	70	GLY	2.2
1	D	195	ARG	2.2
1	D	212	GLY	2.2
1	D	158	PRO	2.2
1	C	302	LEU	2.2
1	D	263	ILE	2.2
1	D	293	GLY	2.2
1	D	199	GLU	2.1
1	C	290	VAL	2.1
1	D	205	ALA	2.1
1	D	264	LEU	2.1
1	D	216	GLU	2.1
1	C	197	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	333	TRP	2.0
1	D	109	VAL	2.0
1	C	86	ILE	2.0
1	C	311	PRO	2.0
1	C	89	TYR	2.0
1	D	215	THR	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, 95th 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^2)	Q<0.9
6	ZN	B	610	1/1	0.01	0.79	520,520,520,520	1
6	ZN	B	609	1/1	0.14	0.15	275,275,275,275	0
6	ZN	A	615	1/1	0.49	0.24	283,283,283,283	0
3	SO4	D	602	5/5	0.57	0.51	188,200,211,233	2
6	ZN	D	607	1/1	0.57	0.47	194,194,194,194	0
4	ACT	D	605	4/4	0.59	0.45	160,163,171,172	1
3	SO4	D	603	5/5	0.60	0.41	212,217,228,233	1
5	EDO	A	610	4/4	0.62	0.62	137,156,171,171	0
6	ZN	C	609	1/1	0.64	0.18	451,451,451,451	0
5	EDO	C	605	4/4	0.65	0.84	127,134,140,140	1
6	ZN	C	608	1/1	0.70	0.16	350,350,350,350	0
6	ZN	C	606	1/1	0.73	0.88	211,211,211,211	0
5	EDO	A	613	4/4	0.74	0.12	142,153,157,159	0
5	EDO	B	606	4/4	0.75	0.58	124,139,141,147	0
3	SO4	A	607	5/5	0.76	0.65	178,192,194,200	1
5	EDO	B	607	4/4	0.76	0.36	116,119,122,128	0
5	EDO	B	604	4/4	0.78	0.28	113,120,131,133	0

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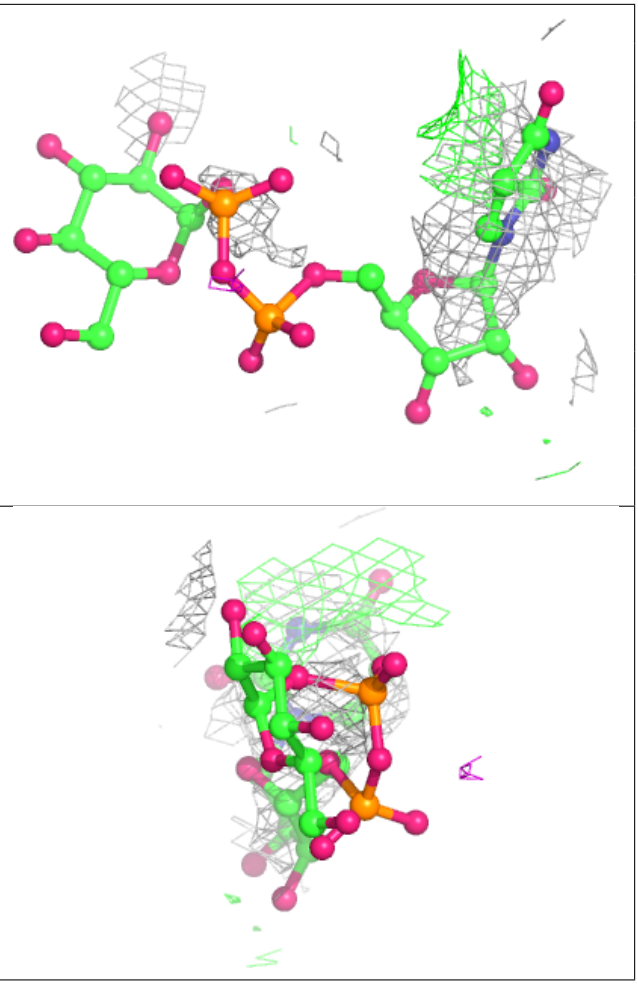
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	605	5/5	0.79	0.13	175,189,208,211	0
2	UPG	A	601	36/36	0.79	0.41	167,268,389,392	17
5	EDO	B	603	4/4	0.80	0.39	89,101,103,117	1
6	ZN	B	608	1/1	0.80	0.16	173,173,173,173	0
3	SO4	C	602	5/5	0.82	0.35	144,168,179,183	0
3	SO4	A	602	5/5	0.85	0.13	197,219,227,243	0
5	EDO	B	605	4/4	0.86	0.25	118,122,125,126	0
4	ACT	A	609	4/4	0.87	0.23	89,90,111,123	0
3	SO4	A	603	5/5	0.87	0.20	171,187,206,215	0
6	ZN	A	614	1/1	0.88	0.42	328,328,328,328	0
4	ACT	C	604	4/4	0.88	0.19	112,129,139,163	0
6	ZN	C	607	1/1	0.88	0.25	147,147,147,147	0
3	SO4	D	601	5/5	0.90	0.11	164,177,193,201	0
4	ACT	D	604	4/4	0.90	0.31	126,144,148,149	0
3	SO4	C	601	5/5	0.90	0.23	137,139,180,186	0
3	SO4	B	601	5/5	0.92	0.19	112,124,153,162	0
3	SO4	A	604	5/5	0.92	0.19	95,116,158,165	0
3	SO4	C	603	5/5	0.93	0.33	142,168,178,187	0
3	SO4	A	608	5/5	0.93	0.18	188,190,212,222	0
3	SO4	B	602	5/5	0.94	0.11	137,167,173,182	0
5	EDO	A	612	4/4	0.95	0.16	85,102,103,106	0
5	EDO	A	611	4/4	0.96	0.28	88,103,111,120	1
3	SO4	A	606	5/5	0.97	0.10	116,142,151,157	0
5	EDO	D	606	4/4	0.97	0.11	132,136,138,140	0
6	ZN	D	608	1/1	0.98	0.12	219,219,219,219	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UPG A 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.