Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 08:59 PM EST

PDB ID	:	1N3L
Title	:	Crystal structure of a human aminoacyl-tRNA synthetase cytokine
Authors	:	Yang, X.-L.; Skene, R.J.; McRee, D.E.; Schimmel, P.
Deposited on	:	2002-10-28
Resolution	:	1.18 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:

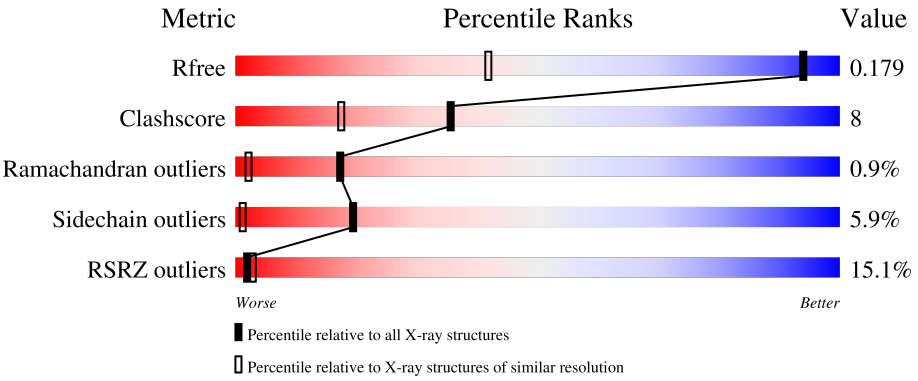
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.18 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	1123 (1.20-1.16)
Clashscore	141614	1182 (1.20-1.16)
Ramachandran outliers	138981	1134 (1.20-1.16)
Sidechain outliers	138945	1134 (1.20-1.16)
RSRZ outliers	127900	1102 (1.20-1.16)

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	372	13% 69% 17% • 11%

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
3	GOL	A	602	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2989 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.

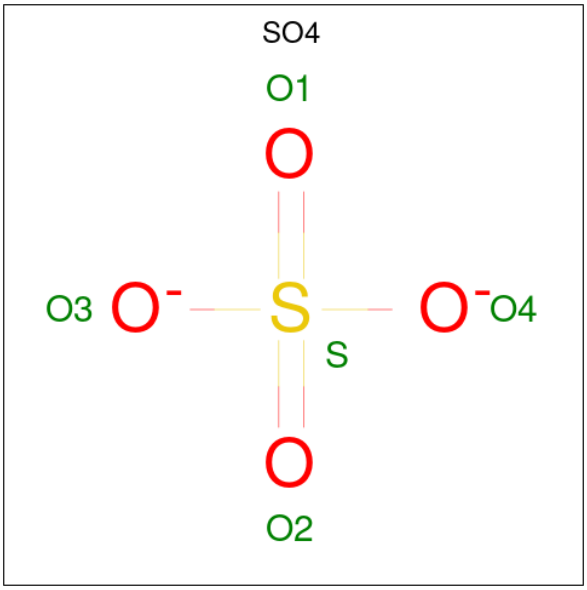
- Molecule 1 is a protein called tyrosyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2641	1714	432	488	7	38	3	0

There are 8 discrepancies between the modelled and reference sequences:

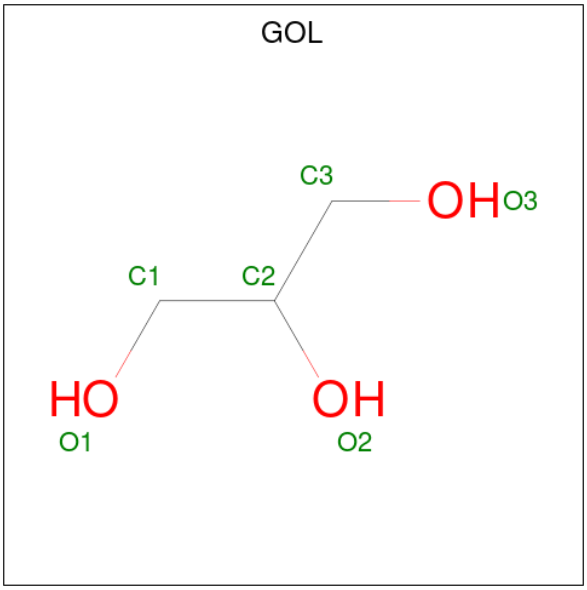
Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LEU	-	expression tag	UNP P54577
A	366	GLU	-	expression tag	UNP P54577
A	367	HIS	-	expression tag	UNP P54577
A	368	HIS	-	expression tag	UNP P54577
A	369	HIS	-	expression tag	UNP P54577
A	370	HIS	-	expression tag	UNP P54577
A	371	HIS	-	expression tag	UNP P54577
A	372	HIS	-	expression tag	UNP P54577

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

- 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

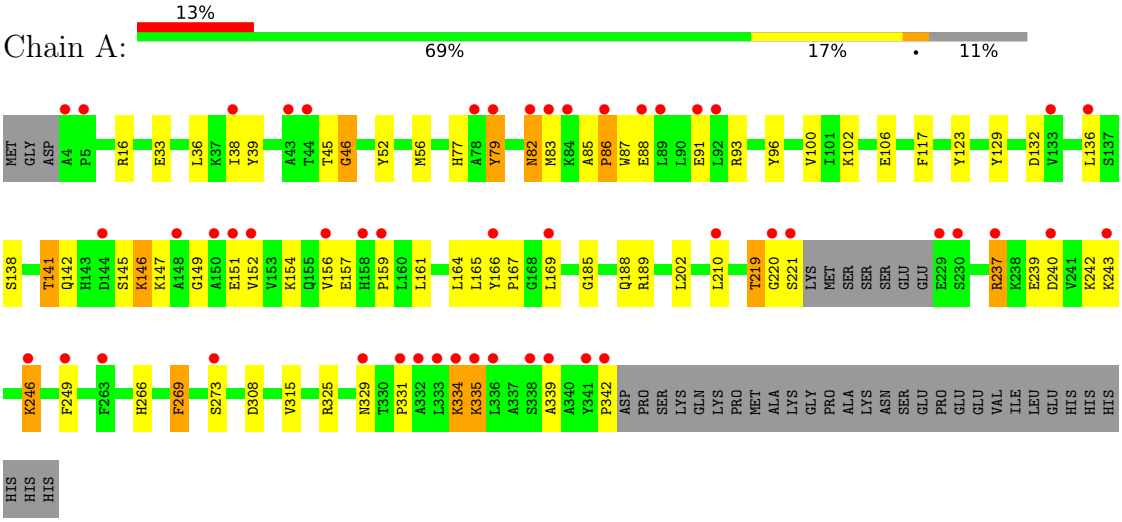
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	316	Total O 316 316	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: tyrosyl-tRNA synthetase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.59Å 162.39Å 35.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.18 29.88 – 1.18	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.18) 86.0 (29.88-1.18)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 1.18Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.180 , 0.223 0.169 , 0.179	Depositor DCC
R_{free} test set	6310 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2989	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: SO4, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.69	0/2709	1.38	25/3658 (0.7%)

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	1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	THR	C-N-CA	17.57	159.19	122.30
1	A	16	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	A	189	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	220	GLY	C-N-CA	7.62	140.74	121.70
1	A	96	TYR	CB-CG-CD2	7.52	125.51	121.00
1	A	132	ASP	CB-CG-OD1	7.13	124.71	118.30
1	A	123	TYR	CB-CG-CD2	7.12	125.27	121.00
1	A	129	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	A	189	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	16	ARG	NH1-CZ-NH2	6.63	126.69	119.40
1	A	79	TYR	CB-CG-CD2	6.56	124.94	121.00
1	A	33	GLU	OE1-CD-OE2	-6.54	115.45	123.30
1	A	161	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	77	HIS	CA-CB-CG	6.03	123.84	113.60
1	A	93	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	308	ASP	CB-CG-OD1	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	TYR	CB-CG-CD1	-5.66	117.60	121.00
1	A	56	MET	CG-SD-CE	5.62	109.20	100.20
1	A	269	PHE	CB-CG-CD2	-5.42	117.01	120.80
1	A	164	LEU	O-C-N	5.33	131.22	122.70
1	A	325	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	117	PHE	CB-CG-CD1	5.16	124.41	120.80
1	A	141	THR	O-C-N	-5.14	114.48	122.70
1	A	52	TYR	CB-CG-CD1	5.09	124.06	121.00
1	A	325	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	THR	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	2641	0	2714	42	0
2	A	20	0	0	0	0
3	A	12	0	16	4	0
4	A	316	0	0	8	0
All	All	2989	0	2730	43	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 8.

All (43) 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:185:GLY:H	1:A:188:GLN:HE21	1.32	0.77
1:A:339:ALA:O	1:A:342:PRO:HD3	1.89	0.73
1:A:266:HIS:NE2	3:A:601:GOL:H31	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ARG:NE	1:A:239:GLU:HB2	2.05	0.71
1:A:142:GLN:O	1:A:146:LYS:HG3	1.91	0.71
1:A:141:THR:HG23	4:A:2226:HOH:O	1.91	0.69
1:A:237:ARG:HD2	1:A:240:ASP:H	1.58	0.69
1:A:157:GLU:O	1:A:159:PRO:HD3	1.98	0.64
3:A:601:GOL:H11	4:A:2146:HOH:O	1.99	0.62
1:A:273:SER:OG	3:A:602:GOL:H12	2.00	0.61
1:A:36:LEU:HD23	1:A:38[B]:ILE:HD11	1.82	0.60
1:A:169:LEU:HD22	4:A:2268:HOH:O	2.01	0.59
1:A:166:TYR:HB3	1:A:167:PRO:HD3	1.86	0.56
1:A:221:SER:HB2	4:A:2070:HOH:O	2.06	0.56
1:A:221:SER:HB3	1:A:249:PHE:CD1	2.42	0.55
1:A:221:SER:HB3	1:A:249:PHE:HB3	1.90	0.54
1:A:82:ASN:O	1:A:85:ALA:HB3	2.07	0.54
1:A:246:LYS:N	1:A:246:LYS:HD3	2.19	0.53
1:A:79:TYR:CZ	1:A:83:MET:HG2	2.45	0.51
1:A:315:VAL:HG23	4:A:2163:HOH:O	2.11	0.51
1:A:149:GLY:O	1:A:151:GLU:O	2.29	0.50
1:A:221:SER:CB	1:A:249:PHE:HB3	2.42	0.49
1:A:38[A]:ILE:CD1	1:A:210:LEU:HD12	2.43	0.48
1:A:331:PRO:O	1:A:335:LYS:HE2	2.13	0.48
1:A:45:THR:O	1:A:46:GLY:O	2.31	0.48
1:A:165:LEU:O	1:A:169:LEU:HG	2.14	0.47
1:A:273:SER:CB	3:A:602:GOL:H12	2.45	0.47
1:A:185:GLY:H	1:A:188:GLN:NE2	2.05	0.46
1:A:169:LEU:HD13	4:A:2268:HOH:O	2.15	0.46
1:A:237:ARG:HD3	1:A:239:GLU:H	1.81	0.46
1:A:237:ARG:HD2	1:A:240:ASP:N	2.28	0.46
1:A:151:GLU:OE1	1:A:151:GLU:N	2.49	0.45
1:A:88:GLU:O	1:A:91:GLU:N	2.50	0.45
1:A:146:LYS:HG3	1:A:146:LYS:H	1.62	0.43
1:A:38[A]:ILE:HD11	1:A:210:LEU:HD12	2.00	0.43
1:A:237:ARG:CD	1:A:239:GLU:HB2	2.49	0.42
1:A:85:ALA:HA	1:A:86:PRO:HD2	1.69	0.42
1:A:237:ARG:HG3	4:A:2171:HOH:O	2.19	0.41
1:A:102:LYS:HE2	1:A:106:GLU:OE2	2.21	0.41
1:A:136:LEU:HG	1:A:202:LEU:HD21	2.03	0.40
1:A:142:GLN:NE2	4:A:2139:HOH:O	2.51	0.40
1:A:151:GLU:O	1:A:152:VAL:HB	2.21	0.40
1:A:334:LYS:HE2	1:A:334:LYS:HB3	1.51	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	331/372 (89%)	313 (95%)	15 (4%)	3 (1%)	17 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	TRP
1	A	86	PRO
1	A	46	GLY

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	289/325 (89%)	271 (94%)	18 (6%)	18 1

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	82	ASN
1	A	100	VAL
1	A	138	SER
1	A	145[A]	SER
1	A	145[B]	SER
1	A	146	LYS
1	A	147	LYS

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Mol	Chain	Res	Type
1	A	154	LYS
1	A	156	VAL
1	A	237	ARG
1	A	242	LYS
1	A	243	LYS
1	A	246	LYS
1	A	269	PHE
1	A	329	ASN
1	A	334	LYS
1	A	335	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	188	GLN
1	A	329	ASN

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)

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	$\#\|Z\| > 2$
3	GOL	A	602	-	5,5,5	0.75	0	5,5,5	1.80	2 (40%)
2	SO4	A	504	-	4,4,4	0.31	0	6,6,6	0.49	0
2	SO4	A	502	-	4,4,4	0.49	0	6,6,6	0.43	0
3	GOL	A	601	-	5,5,5	0.62	0	5,5,5	1.80	1 (20%)
2	SO4	A	503	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	A	501	-	4,4,4	0.40	0	6,6,6	0.45	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	602	-	-	4/4/4/4	-
3	GOL	A	601	-	-	3/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	GOL	O3-C3-C2	3.06	124.87	110.20
3	A	602	GOL	O1-C1-C2	-2.86	96.49	110.20
3	A	602	GOL	O2-C2-C1	-2.58	97.77	109.12

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-O2
3	A	601	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	GOL	2	0
3	A	601	GOL	2	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^{th} 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	332/372 (89%)	0.76	50 (15%)	2 3	15, 24, 57, 75	23 (6%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	GLY	7.9
1	A	221	SER	6.5
1	A	156	VAL	6.3
1	A	84	LYS	6.0
1	A	335	LYS	5.4
1	A	88	GLU	4.9
1	A	150	ALA	4.8
1	A	158	HIS	4.7
1	A	4	ALA	4.4
1	A	342	PRO	4.4
1	A	83	MET	4.3
1	A	86	PRO	4.2
1	A	237	ARG	4.1
1	A	341	TYR	4.0
1	A	249	PHE	3.9
1	A	92	LEU	3.8
1	A	152	VAL	3.7
1	A	246	LYS	3.7
1	A	334	LYS	3.7
1	A	243	LYS	3.5
1	A	331	PRO	3.4
1	A	44	THR	3.4
1	A	79	TYR	3.2
1	A	230	SER	3.2
1	A	332	ALA	3.2
1	A	82	ASN	3.1
1	A	38[A]	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	151	GLU	3.0
1	A	169	LEU	2.9
1	A	338	SER	2.9
1	A	91	GLU	2.9
1	A	5	PRO	2.8
1	A	136	LEU	2.8
1	A	159	PRO	2.7
1	A	229	GLU	2.6
1	A	339	ALA	2.6
1	A	166	TYR	2.6
1	A	329	ASN	2.5
1	A	78	ALA	2.5
1	A	133	VAL	2.4
1	A	148	ALA	2.4
1	A	263	PHE	2.4
1	A	336	LEU	2.3
1	A	210	LEU	2.3
1	A	273	SER	2.2
1	A	89	LEU	2.2
1	A	333	LEU	2.2
1	A	240	ASP	2.1
1	A	43	ALA	2.1
1	A	144	ASP	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	503	5/5	0.78	0.17	47,70,72,74	5
3	GOL	A	601	6/6	0.82	0.18	33,39,47,53	0
3	GOL	A	602	6/6	0.88	0.15	41,49,56,64	0
2	SO4	A	504	5/5	0.95	0.20	40,56,62,70	0
2	SO4	A	502	5/5	0.97	0.21	33,36,44,64	0
2	SO4	A	501	5/5	0.99	0.06	22,23,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.