



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 01:06 PM EST

PDB ID : 4REF
Title : Crystal Structure of TR3 LBD_L449W in complex with Molecule 2
Authors : Li, F.W.; Cai, Q.X.; Li, A.Z.; Tian, X.Y.; Wang, W.J.; Yuan, W.; Hou, P.P.;
Wu, Q.; Lin, T.W.
Deposited on : unknown
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (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

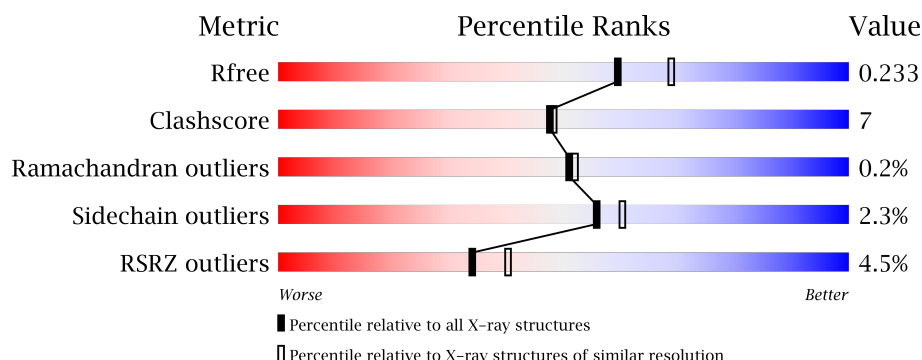
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 ≥ 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	256	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>
1	B	256	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>8%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	303	-	-	-	X
3	3N0	A	302	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4004 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 Nuclear receptor subfamily 4 group A member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	235	Total	C	N	O	S	0	0	0
			1827	1180	311	329	7			
1	A	231	Total	C	N	O	S	0	0	0
			1822	1180	310	325	7			

There are 18 discrepancies between the modelled and reference sequences:

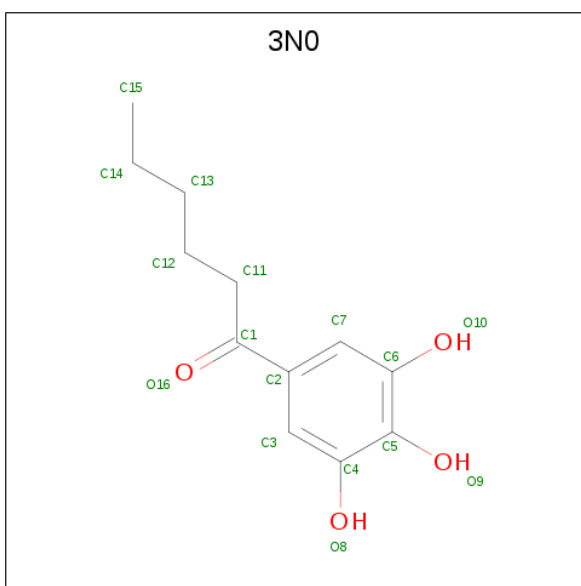
Chain	Residue	Modelled	Actual	Comment	Reference
B	118	TRP	LEU	ENGINEERED MUTATION	UNP P22736
B	268	LEU	-	EXPRESSION TAG	UNP P22736
B	269	GLU	-	EXPRESSION TAG	UNP P22736
B	270	HIS	-	EXPRESSION TAG	UNP P22736
B	271	HIS	-	EXPRESSION TAG	UNP P22736
B	272	HIS	-	EXPRESSION TAG	UNP P22736
B	273	HIS	-	EXPRESSION TAG	UNP P22736
B	274	HIS	-	EXPRESSION TAG	UNP P22736
B	275	HIS	-	EXPRESSION TAG	UNP P22736
A	118	TRP	LEU	ENGINEERED MUTATION	UNP P22736
A	268	LEU	-	EXPRESSION TAG	UNP P22736
A	269	GLU	-	EXPRESSION TAG	UNP P22736
A	270	HIS	-	EXPRESSION TAG	UNP P22736
A	271	HIS	-	EXPRESSION TAG	UNP P22736
A	272	HIS	-	EXPRESSION TAG	UNP P22736
A	273	HIS	-	EXPRESSION TAG	UNP P22736
A	274	HIS	-	EXPRESSION TAG	UNP P22736
A	275	HIS	-	EXPRESSION TAG	UNP P22736

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is 1-(3,4,5-trihydroxyphenyl)hexan-1-one (three-letter code: 3N0) (formula: $C_{12}H_{16}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	12	4		

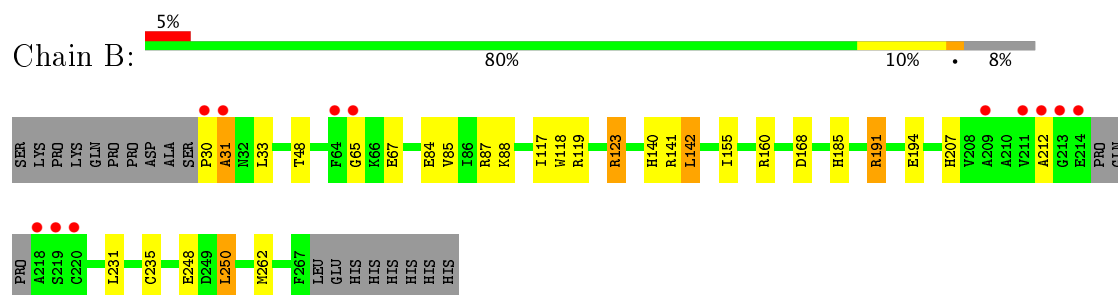
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	158	Total	O	0	0
			158	158		
4	A	157	Total	O	0	0
			157	157		

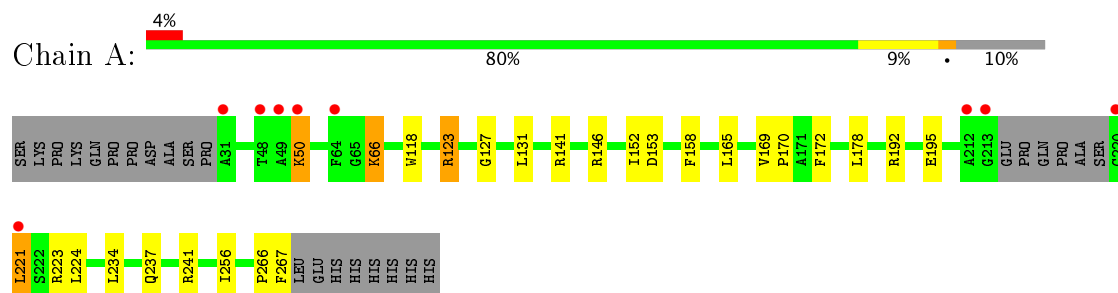
3 Residue-property plots [i](#)

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: Nuclear receptor subfamily 4 group A member 1



- Molecule 1: Nuclear receptor subfamily 4 group A member 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.20Å 76.84Å 128.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.03 – 2.10 37.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.03-2.10) 98.9 (37.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.187 , 0.230 0.195 , 0.233	Depositor DCC
R_{free} test set	2150 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4004	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 3N0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	1/1862 (0.1%)	1.08	5/2522 (0.2%)
1	B	1.00	1/1867 (0.1%)	1.15	7/2532 (0.3%)
All	All	1.00	2/3729 (0.1%)	1.12	12/5054 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	ARG	CD-NE	-6.20	1.35	1.46
1	A	123	ARG	CD-NE	-5.81	1.36	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ARG	NE-CZ-NH2	-24.85	107.88	120.30
1	A	123	ARG	NE-CZ-NH2	-23.16	108.72	120.30
1	B	123	ARG	NE-CZ-NH1	19.48	130.04	120.30
1	A	123	ARG	NE-CZ-NH1	18.10	129.35	120.30
1	A	192	ARG	NE-CZ-NH2	8.67	124.64	120.30
1	B	123	ARG	CD-NE-CZ	8.12	134.97	123.60
1	A	123	ARG	CD-NE-CZ	7.62	134.27	123.60
1	B	168	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	119	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	65	GLY	N-CA-C	5.62	127.15	113.10
1	A	241	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	235	CYS	CA-CB-SG	-5.38	104.32	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1822	0	1863	32	0
1	B	1827	0	1845	20	0
2	A	18	0	24	3	0
2	B	6	0	8	2	0
3	A	16	0	15	1	0
4	A	157	0	0	6	0
4	B	158	0	0	8	0
All	All	4004	0	3755	52	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 7.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH2	1:B:194:GLU:OE1	1.80	1.13
1:B:87:ARG:NH1	4:B:449:HOH:O	1.90	1.03
1:A:50:LYS:NZ	1:A:50:LYS:O	2.02	0.93
1:A:221:LEU:HD11	1:A:223:ARG:HB2	1.52	0.91
1:A:221:LEU:CD1	1:A:223:ARG:HB2	2.01	0.90
1:B:30:PRO:HB2	1:B:31:ALA:CA	2.13	0.78
1:A:221:LEU:HD12	1:A:224:LEU:H	1.47	0.78
1:B:84:GLU:OE2	1:B:88:LYS:NZ	2.18	0.77
1:B:191:ARG:HH21	1:B:194:GLU:CD	1.90	0.75
1:B:207:HIS:HD2	4:B:429:HOH:O	1.68	0.75
1:A:221:LEU:HD12	1:A:223:ARG:N	2.07	0.70
1:B:262:MET:CE	4:B:458:HOH:O	2.40	0.68
1:B:212:ALA:HA	4:B:547:HOH:O	1.94	0.68
1:B:191:ARG:HA	1:B:194:GLU:HG2	1.77	0.66
1:B:248:GLU:HG2	1:B:250:LEU:HD13	1.78	0.65
1:B:123:ARG:HD3	2:B:301:GOL:O2	1.97	0.64
1:A:256:ILE:HG23	4:A:459:HOH:O	1.99	0.63
1:A:127:GLY:H	2:A:303:GOL:H31	1.66	0.61
1:B:85:VAL:HG23	4:B:453:HOH:O	2.02	0.58
1:A:123:ARG:HD3	2:A:301:GOL:O2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:MET:HE3	4:B:458:HOH:O	2.03	0.56
1:A:127:GLY:N	2:A:303:GOL:H31	2.23	0.54
1:A:221:LEU:HD11	4:A:436:HOH:O	2.07	0.54
1:A:66:LYS:HD2	1:A:146:ARG:HH22	1.73	0.53
1:B:141:ARG:NH2	1:B:142:LEU:HD11	2.24	0.53
1:A:66:LYS:HD2	1:A:146:ARG:NH2	2.24	0.52
1:A:66:LYS:HG3	1:A:146:ARG:NH1	2.25	0.51
1:A:221:LEU:CD1	1:A:224:LEU:H	2.19	0.51
1:A:237:GLN:HG2	4:A:553:HOH:O	2.11	0.51
1:B:30:PRO:N	1:B:33:LEU:H	2.07	0.51
1:A:221:LEU:CD1	1:A:223:ARG:N	2.74	0.51
1:A:141:ARG:HD2	1:A:153:ASP:OD1	2.12	0.50
1:A:221:LEU:CD1	1:A:223:ARG:H	2.25	0.50
1:A:221:LEU:HD12	1:A:224:LEU:N	2.23	0.49
1:A:221:LEU:CD1	1:A:223:ARG:CB	2.85	0.48
1:A:178:LEU:HB3	3:A:302:3N0:H1	1.96	0.47
1:A:131:LEU:HG	1:A:152:ILE:HD11	1.98	0.46
1:B:185:HIS:HD2	4:B:502:HOH:O	1.99	0.45
1:A:221:LEU:C	1:A:221:LEU:CD1	2.85	0.45
1:A:195:GLU:OE1	4:A:490:HOH:O	2.21	0.45
1:B:160:ARG:NH1	4:B:430:HOH:O	2.50	0.45
1:A:165:LEU:HD22	4:A:436:HOH:O	2.17	0.44
1:A:158:PHE:HB2	1:A:234:LEU:HD11	1.99	0.44
1:A:221:LEU:HD21	4:A:536:HOH:O	2.17	0.44
1:A:266:PRO:O	1:A:267:PHE:HB3	2.17	0.44
1:A:66:LYS:HG3	1:A:146:ARG:HH12	1.82	0.43
1:B:123:ARG:CD	2:B:301:GOL:O2	2.67	0.43
1:B:118:TRP:HB2	1:B:231:LEU:HD21	2.01	0.42
1:A:118:TRP:CE2	1:A:172:PHE:CE1	3.08	0.42
1:A:169:VAL:HB	1:A:170:PRO:HD3	2.03	0.41
1:B:117:ILE:HD12	1:B:155:ILE:CD1	2.52	0.40
1:A:66:LYS:CG	1:A:146:ARG:HH12	2.34	0.40

There are no symmetry-related clashes.

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	227/256 (89%)	223 (98%)	4 (2%)	0	100	100
1	B	231/256 (90%)	226 (98%)	4 (2%)	1 (0%)	38	35
All	All	458/512 (90%)	449 (98%)	8 (2%)	1 (0%)	51	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	ALA

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	199/222 (90%)	196 (98%)	3 (2%)	70	76
1	B	197/222 (89%)	191 (97%)	6 (3%)	46	49
All	All	396/444 (89%)	387 (98%)	9 (2%)	56	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	48	THR
1	B	67	GLU
1	B	140	HIS
1	B	142	LEU
1	B	191	ARG
1	B	250	LEU
1	A	50	LYS
1	A	66	LYS
1	A	221	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	104	GLN
1	A	104	GLN

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 ⓘ

5 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	GOL	A	301	-	5,5,5	0.46	0	5,5,5	0.42	0
3	3N0	A	302	-	16,16,16	0.80	0	21,21,21	2.05	5 (23%)
2	GOL	A	303	-	5,5,5	0.88	0	5,5,5	1.41	0
2	GOL	A	304	-	5,5,5	0.30	0	5,5,5	0.62	0
2	GOL	B	301	-	5,5,5	0.55	0	5,5,5	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	301	-	-	0/4/4/4	0/0/0/0
3	3N0	A	302	-	-	0/9/9/9	0/1/1/1
2	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	GOL	A	304	-	-	0/4/4/4	0/0/0/0
2	GOL	B	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	3N0	C3-C4-C5	-3.93	117.77	120.45
3	A	302	3N0	C7-C6-C5	-2.94	118.44	120.45
3	A	302	3N0	O16-C1-C2	-2.53	116.97	120.74
3	A	302	3N0	C6-C5-C4	3.95	122.03	119.50
3	A	302	3N0	C11-C1-C2	4.60	125.83	119.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GOL	1	0
3	A	302	3N0	1	0
2	A	303	GOL	2	0
2	B	301	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, 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	231/256 (90%)	-0.24	9 (3%) 40 47	21, 33, 62, 101	1 (0%)
1	B	235/256 (91%)	-0.19	12 (5%) 29 35	21, 33, 65, 124	0
All	All	466/512 (91%)	-0.21	21 (4%) 34 40	21, 33, 65, 124	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	GLY	8.2
1	B	212	ALA	6.9
1	B	214	GLU	6.6
1	B	30	PRO	5.6
1	B	65	GLY	5.4
1	A	212	ALA	4.9
1	A	49	ALA	4.8
1	B	219	SER	4.4
1	A	220	CYS	4.2
1	B	31	ALA	3.8
1	A	213	GLY	3.7
1	B	218	ALA	3.7
1	B	220	CYS	3.7
1	A	221	LEU	3.2
1	B	211	VAL	2.8
1	A	31	ALA	2.8
1	A	50	LYS	2.7
1	B	64	PHE	2.5
1	B	209	ALA	2.4
1	A	64	PHE	2.1
1	A	48	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 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	3N0	A	302	16/16	0.76	0.25	8.17	46,76,98,99	0
2	GOL	A	303	6/6	0.80	0.18	6.85	35,51,60,62	0
2	GOL	A	304	6/6	0.89	0.12	0.34	52,58,64,70	0
2	GOL	B	301	6/6	0.97	0.09	-0.65	25,29,30,33	0
2	GOL	A	301	6/6	0.97	0.06	-0.90	28,31,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.