WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:30 am GMT

PDB ID	:	3WT1
Title	:	Crystal structure of the b'-a' domain of thermophilic fungal protein disulfide isomerase (reduced form)
Authors	:	Inagaki, K.; Satoh, T.; Itoh, S.G.; Okumura, H.; Kato, K.
Deposited on	:	2014-04-02
Resolution	:	1.85 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:

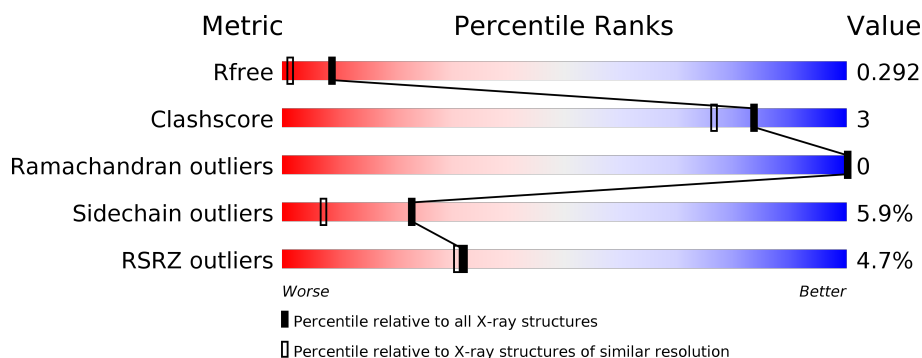|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 1.85 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	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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 <=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	247	
1	B	247	
1	C	247	
1	D	247	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	501	-	-	-	X
2	GOL	B	501	-	-	-	X
2	GOL	C	501	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7831 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 Protein disulfide-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	2	0
			1901	1227	304	367	3			
1	B	242	Total	C	N	O	S	0	0	0
			1878	1214	299	362	3			
1	C	242	Total	C	N	O	S	0	1	0
			1883	1217	299	364	3			
1	D	242	Total	C	N	O	S	0	1	0
			1883	1217	299	364	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	GLY	-	EXPRESSION TAG	UNP P55059
A	204	PRO	-	EXPRESSION TAG	UNP P55059
A	205	LEU	-	EXPRESSION TAG	UNP P55059
A	206	GLY	-	EXPRESSION TAG	UNP P55059
A	207	SER	-	EXPRESSION TAG	UNP P55059
B	203	GLY	-	EXPRESSION TAG	UNP P55059
B	204	PRO	-	EXPRESSION TAG	UNP P55059
B	205	LEU	-	EXPRESSION TAG	UNP P55059
B	206	GLY	-	EXPRESSION TAG	UNP P55059
B	207	SER	-	EXPRESSION TAG	UNP P55059
C	203	GLY	-	EXPRESSION TAG	UNP P55059
C	204	PRO	-	EXPRESSION TAG	UNP P55059
C	205	LEU	-	EXPRESSION TAG	UNP P55059
C	206	GLY	-	EXPRESSION TAG	UNP P55059
C	207	SER	-	EXPRESSION TAG	UNP P55059
D	203	GLY	-	EXPRESSION TAG	UNP P55059
D	204	PRO	-	EXPRESSION TAG	UNP P55059
D	205	LEU	-	EXPRESSION TAG	UNP P55059
D	206	GLY	-	EXPRESSION TAG	UNP P55059
D	207	SER	-	EXPRESSION TAG	UNP P55059

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 3 is water.

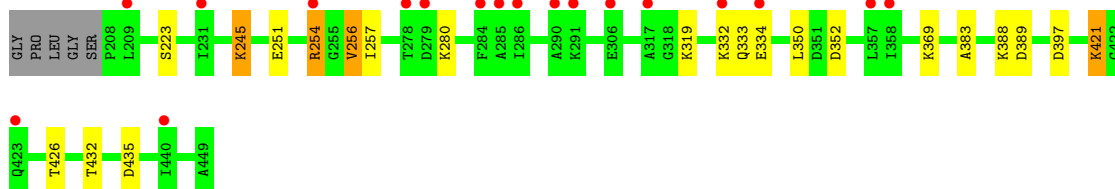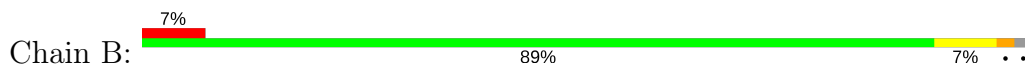| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total 75	O 75	0	0
3	B	45	Total 45	O 45	0	0
3	C	79	Total 79	O 79	0	0
3	D	63	Total 63	O 63	0	0

3 Residue-property plots ⓘ

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.
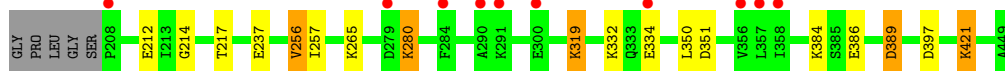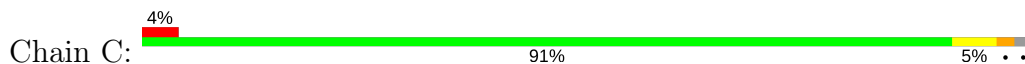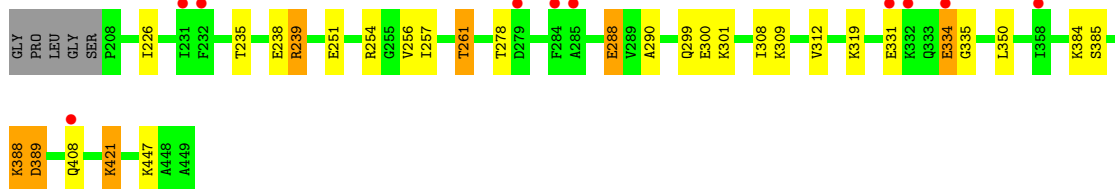
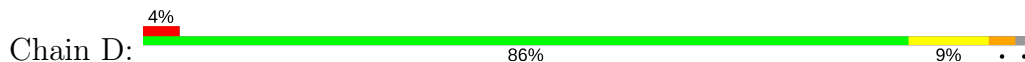- Molecule 1: Protein disulfide-isomerase

Chain A:

- Molecule 1: Protein disulfide-isomerase

Chain B:

- Molecule 1: Protein disulfide-isomerase

Chain C:

- Molecule 1: Protein disulfide-isomerase

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.77Å 67.75Å 70.25Å 105.92° 113.13° 96.59°	Depositor
Resolution (Å)	20.00 – 1.85 19.97 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.1 (20.00-1.85) 81.3 (19.97-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.238 , 0.278 0.250 , 0.292	Depositor DCC
R_{free} test set	4080 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.7	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7831	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.83	0/1950	0.84	3/2641 (0.1%)
1	B	0.67	0/1921	0.79	3/2602 (0.1%)
1	C	0.78	0/1929	0.85	5/2613 (0.2%)
1	D	0.74	0/1929	0.83	4/2613 (0.2%)
All	All	0.76	0/7729	0.83	15/10469 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	389[A]	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	389[B]	ASP	CB-CG-OD1	7.00	124.60	118.30
1	C	389[A]	ASP	CB-CG-OD1	6.92	124.53	118.30
1	C	389[B]	ASP	CB-CG-OD1	6.92	124.53	118.30
1	D	389[A]	ASP	CB-CG-OD1	6.71	124.34	118.30
1	D	389[B]	ASP	CB-CG-OD1	6.71	124.34	118.30
1	C	389[A]	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	389[B]	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	D	239	ARG	CG-CD-NE	5.58	123.52	111.80
1	B	389	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	D	239	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	209	LEU	CA-CB-CG	5.26	127.40	115.30
1	C	397	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	397	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	352	ASP	CB-CG-OD1	5.15	122.93	118.30

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	1901	0	1896	12	0
1	B	1878	0	1872	9	0
1	C	1883	0	1876	9	0
1	D	1883	0	1876	14	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	75	0	0	2	0
3	B	45	0	0	1	0
3	C	79	0	0	0	0
3	D	63	0	0	1	0
All	All	7831	0	7552	42	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 3.

All (42) 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:212:GLU:O	1:C:217:THR:HG21	1.53	1.07
1:B:432:THR:HG23	1:B:435:ASP:H	1.48	0.78
1:C:280:LYS:HA	1:C:280:LYS:HE2	1.72	0.71
1:D:235:THR:HG23	1:D:238:GLU:H	1.59	0.68
1:B:383:ALA:O	1:B:388:LYS:HG3	1.94	0.67
1:D:239:ARG:HD2	1:D:261:THR:HG23	1.79	0.64
1:D:447:LYS:NZ	3:D:629:HOH:O	2.28	0.63
1:C:319:LYS:O	1:C:319:LYS:HD2	1.99	0.62
1:B:426:THR:HG23	3:B:640:HOH:O	1.99	0.62
1:D:251:GLU:OE2	1:D:254:ARG:NH1	2.32	0.60
1:A:383:ALA:O	1:A:388:LYS:HG3	2.05	0.56
1:C:214:GLY:H	1:C:217:THR:HG22	1.71	0.55
1:B:223:SER:HB3	1:D:226:ILE:HG22	1.90	0.54
1:A:432:THR:HG22	1:A:435:ASP:CB	2.39	0.53
1:A:432:THR:CG2	1:A:435:ASP:H	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:THR:HA	3:A:661:HOH:O	2.10	0.52
1:A:331:GLU:HG2	1:A:332:LYS:HG3	1.92	0.51
1:B:251:GLU:O	1:B:254:ARG:HG2	2.10	0.51
1:A:432:THR:HG22	1:A:435:ASP:HB2	1.92	0.49
1:C:350:LEU:HA	1:C:421:LYS:HG2	1.96	0.48
1:A:331:GLU:HG2	1:A:332:LYS:CD	2.44	0.47
1:B:350:LEU:HA	1:B:421:LYS:HG2	1.96	0.47
1:A:350:LEU:HA	1:A:421:LYS:HG2	1.96	0.47
1:D:334:GLU:HG3	1:D:335:GLY:N	2.30	0.46
1:C:256:VAL:HG22	1:C:257:ILE:HG13	1.97	0.46
1:D:350:LEU:HA	1:D:421:LYS:HG2	1.98	0.46
1:A:432:THR:HG22	1:A:435:ASP:H	1.81	0.46
1:B:256:VAL:HG22	1:B:257:ILE:HG13	1.98	0.45
1:D:256:VAL:HG12	1:D:257:ILE:HG13	1.98	0.45
1:A:256:VAL:HG22	1:A:257:ILE:HG13	1.98	0.45
1:D:308:ILE:O	1:D:312:VAL:HG12	2.16	0.45
1:D:239:ARG:HD2	1:D:261:THR:CG2	2.45	0.45
1:C:386:GLU:CD	1:C:386:GLU:H	2.20	0.44
1:D:385:SER:O	1:D:388:LYS:HD2	2.19	0.43
1:B:223:SER:CB	1:D:226:ILE:HG22	2.47	0.42
1:D:309:LYS:HA	1:D:312:VAL:HG12	1.99	0.42
1:A:447:LYS:HE3	3:A:674:HOH:O	2.18	0.42
1:D:288:GLU:HG3	1:D:290:ALA:O	2.20	0.42
1:C:351:ASP:C	1:C:351:ASP:OD1	2.58	0.42
1:A:331:GLU:HG2	1:A:332:LYS:HD3	2.03	0.41
1:C:214:GLY:H	1:C:217:THR:CG2	2.31	0.41
1:B:245:LYS:HD3	1:B:245:LYS:HA	1.91	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	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
1	B	240/247 (97%)	237 (99%)	3 (1%)	0	100	100
1	C	241/247 (98%)	238 (99%)	3 (1%)	0	100	100
1	D	241/247 (98%)	236 (98%)	5 (2%)	0	100	100
All	All	966/988 (98%)	952 (99%)	14 (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	199/199 (100%)	186 (94%)	13 (6%)	20	5
1	B	196/199 (98%)	186 (95%)	10 (5%)	28	10
1	C	197/199 (99%)	186 (94%)	11 (6%)	25	8
1	D	197/199 (99%)	182 (92%)	15 (8%)	15	3
All	All	789/796 (99%)	740 (94%)	49 (6%)	23	6

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	LEU
1	A	256	VAL
1	A	261	THR
1	A	278	THR
1	A	280	LYS
1	A	319	LYS
1	A	332	LYS
1	A	333	GLN
1	A	369	LYS
1	A	389[A]	ASP
1	A	389[B]	ASP
1	A	421	LYS
1	A	432	THR

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Mol	Chain	Res	Type
1	B	245	LYS
1	B	254	ARG
1	B	256	VAL
1	B	280	LYS
1	B	319	LYS
1	B	332	LYS
1	B	333	GLN
1	B	334	GLU
1	B	369	LYS
1	B	421	LYS
1	C	237	GLU
1	C	256	VAL
1	C	265	LYS
1	C	280	LYS
1	C	319	LYS
1	C	332	LYS
1	C	334	GLU
1	C	384	LYS
1	C	389[A]	ASP
1	C	389[B]	ASP
1	C	421	LYS
1	D	261	THR
1	D	278	THR
1	D	288	GLU
1	D	299	GLN
1	D	300	GLU
1	D	301	LYS
1	D	319	LYS
1	D	331	GLU
1	D	334	GLU
1	D	384	LYS
1	D	388	LYS
1	D	389[A]	ASP
1	D	389[B]	ASP
1	D	408	GLN
1	D	421	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	258	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 ⓘ

4 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	501	-	5,5,5	1.09	0	5,5,5	1.21	0
2	GOL	B	501	-	5,5,5	1.06	0	5,5,5	1.24	0
2	GOL	C	501	-	5,5,5	1.09	0	5,5,5	1.57	2 (40%)
2	GOL	D	501	-	5,5,5	1.21	0	5,5,5	1.27	1 (20%)

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	501	-	-	0/4/4/4	0/0/0/0
2	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	501	-	-	0/4/4/4	0/0/0/0
2	GOL	D	501	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	GOL	O3-C3-C2	2.04	120.34	110.07
2	C	501	GOL	O1-C1-C2	2.09	120.62	110.07
2	C	501	GOL	C3-C2-C1	2.14	120.01	111.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	244/247 (98%)	0.08	8 (3%)	47	45	21, 35, 60, 82	0
1	B	242/247 (97%)	0.34	18 (7%)	15	15	28, 42, 65, 87	0
1	C	242/247 (97%)	0.22	10 (4%)	38	36	23, 37, 65, 88	0
1	D	242/247 (97%)	0.25	10 (4%)	38	36	23, 40, 62, 80	0
All	All	970/988 (98%)	0.22	46 (4%)	32	31	21, 39, 63, 88	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	334	GLU	4.5
1	B	334	GLU	3.9
1	B	358	ILE	3.8
1	D	358	ILE	3.7
1	B	290	ALA	3.5
1	A	284	PHE	3.4
1	C	357	LEU	3.3
1	D	408	GLN	3.2
1	B	291	LYS	3.2
1	B	209	LEU	3.1
1	C	284	PHE	3.1
1	B	284	PHE	3.1
1	D	334	GLU	3.0
1	A	290	ALA	3.0
1	B	357	LEU	2.9
1	C	358	ILE	2.9
1	A	333	GLN	2.9
1	C	208	PRO	2.9
1	D	231	ILE	2.9
1	D	284	PHE	2.8
1	A	334	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	278	THR	2.7
1	B	285	ALA	2.7
1	C	279	ASP	2.7
1	B	332	LYS	2.6
1	A	286	ILE	2.4
1	B	278	THR	2.4
1	B	317	ALA	2.4
1	A	408	GLN	2.4
1	D	331	GLU	2.4
1	C	291	LYS	2.4
1	B	306	GLU	2.3
1	B	231	ILE	2.3
1	B	286	ILE	2.3
1	A	357	LEU	2.3
1	B	423	GLN	2.2
1	D	285	ALA	2.2
1	D	279	ASP	2.2
1	C	290	ALA	2.2
1	C	356	VAL	2.2
1	B	279	ASP	2.1
1	D	232	PHE	2.1
1	D	332	LYS	2.1
1	B	440	ILE	2.1
1	B	254	ARG	2.0
1	C	300	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
2	GOL	C	501	6/6	0.85	0.18	4.87	33,36,40,42	0
2	GOL	B	501	6/6	0.90	0.20	3.87	45,48,50,58	0
2	GOL	A	501	6/6	0.79	0.22	3.19	33,40,53,54	0
2	GOL	D	501	6/6	0.80	0.15	0.81	35,38,40,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.