W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 07:05 pm BST

PDB ID	:	3PG6
Title	:	The carboxyl terminal domain of human deltex 3-like
Authors	:	Walker, J.R.; Obiero, J.; Kania, J.; Schuler, H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Arrowsmith, C.H.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on	:	2010-10-30
Resolution	:	1.70 Å(reported)

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

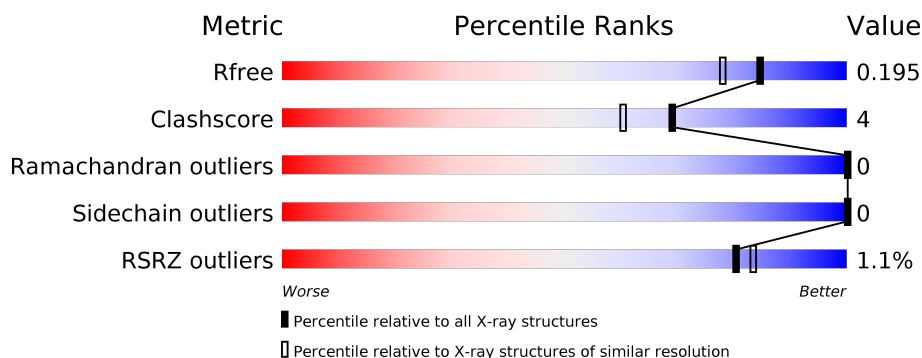|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.195
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		1.1%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	159	2% / 79% 6% 15%
1	B	159	% / 75% 9% 16%
1	C	159	% / 80% 5% 15%
1	D	159	81% • 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5113 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 E3 ubiquitin-protein ligase DTX3L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	3	0
			1089	699	182	205	3			
1	B	134	Total	C	N	O	S	0	7	0
			1121	712	192	214	3			
1	C	135	Total	C	N	O	S	0	5	0
			1109	710	192	204	3			
1	D	134	Total	C	N	O	S	0	5	0
			1093	702	183	205	3			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	582	MET	-	EXPRESSION TAG	UNP Q8TDB6
A	583	GLY	-	EXPRESSION TAG	UNP Q8TDB6
A	584	SER	-	EXPRESSION TAG	UNP Q8TDB6
A	585	SER	-	EXPRESSION TAG	UNP Q8TDB6
A	586	HIS	-	EXPRESSION TAG	UNP Q8TDB6
A	587	HIS	-	EXPRESSION TAG	UNP Q8TDB6
A	588	HIS	-	EXPRESSION TAG	UNP Q8TDB6
A	589	HIS	-	EXPRESSION TAG	UNP Q8TDB6
A	590	HIS	-	EXPRESSION TAG	UNP Q8TDB6
A	591	HIS	-	EXPRESSION TAG	UNP Q8TDB6
A	592	SER	-	EXPRESSION TAG	UNP Q8TDB6
A	593	SER	-	EXPRESSION TAG	UNP Q8TDB6
A	594	GLY	-	EXPRESSION TAG	UNP Q8TDB6
A	595	LEU	-	EXPRESSION TAG	UNP Q8TDB6
A	596	VAL	-	EXPRESSION TAG	UNP Q8TDB6
A	597	PRO	-	EXPRESSION TAG	UNP Q8TDB6
A	598	ARG	-	EXPRESSION TAG	UNP Q8TDB6
A	599	GLY	-	EXPRESSION TAG	UNP Q8TDB6
A	600	SER	-	EXPRESSION TAG	UNP Q8TDB6
B	582	MET	-	EXPRESSION TAG	UNP Q8TDB6
B	583	GLY	-	EXPRESSION TAG	UNP Q8TDB6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	584	SER	-	EXPRESSION TAG	UNP Q8TDB6
B	585	SER	-	EXPRESSION TAG	UNP Q8TDB6
B	586	HIS	-	EXPRESSION TAG	UNP Q8TDB6
B	587	HIS	-	EXPRESSION TAG	UNP Q8TDB6
B	588	HIS	-	EXPRESSION TAG	UNP Q8TDB6
B	589	HIS	-	EXPRESSION TAG	UNP Q8TDB6
B	590	HIS	-	EXPRESSION TAG	UNP Q8TDB6
B	591	HIS	-	EXPRESSION TAG	UNP Q8TDB6
B	592	SER	-	EXPRESSION TAG	UNP Q8TDB6
B	593	SER	-	EXPRESSION TAG	UNP Q8TDB6
B	594	GLY	-	EXPRESSION TAG	UNP Q8TDB6
B	595	LEU	-	EXPRESSION TAG	UNP Q8TDB6
B	596	VAL	-	EXPRESSION TAG	UNP Q8TDB6
B	597	PRO	-	EXPRESSION TAG	UNP Q8TDB6
B	598	ARG	-	EXPRESSION TAG	UNP Q8TDB6
B	599	GLY	-	EXPRESSION TAG	UNP Q8TDB6
B	600	SER	-	EXPRESSION TAG	UNP Q8TDB6
C	582	MET	-	EXPRESSION TAG	UNP Q8TDB6
C	583	GLY	-	EXPRESSION TAG	UNP Q8TDB6
C	584	SER	-	EXPRESSION TAG	UNP Q8TDB6
C	585	SER	-	EXPRESSION TAG	UNP Q8TDB6
C	586	HIS	-	EXPRESSION TAG	UNP Q8TDB6
C	587	HIS	-	EXPRESSION TAG	UNP Q8TDB6
C	588	HIS	-	EXPRESSION TAG	UNP Q8TDB6
C	589	HIS	-	EXPRESSION TAG	UNP Q8TDB6
C	590	HIS	-	EXPRESSION TAG	UNP Q8TDB6
C	591	HIS	-	EXPRESSION TAG	UNP Q8TDB6
C	592	SER	-	EXPRESSION TAG	UNP Q8TDB6
C	593	SER	-	EXPRESSION TAG	UNP Q8TDB6
C	594	GLY	-	EXPRESSION TAG	UNP Q8TDB6
C	595	LEU	-	EXPRESSION TAG	UNP Q8TDB6
C	596	VAL	-	EXPRESSION TAG	UNP Q8TDB6
C	597	PRO	-	EXPRESSION TAG	UNP Q8TDB6
C	598	ARG	-	EXPRESSION TAG	UNP Q8TDB6
C	599	GLY	-	EXPRESSION TAG	UNP Q8TDB6
C	600	SER	-	EXPRESSION TAG	UNP Q8TDB6
D	582	MET	-	EXPRESSION TAG	UNP Q8TDB6
D	583	GLY	-	EXPRESSION TAG	UNP Q8TDB6
D	584	SER	-	EXPRESSION TAG	UNP Q8TDB6
D	585	SER	-	EXPRESSION TAG	UNP Q8TDB6
D	586	HIS	-	EXPRESSION TAG	UNP Q8TDB6
D	587	HIS	-	EXPRESSION TAG	UNP Q8TDB6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	588	HIS	-	EXPRESSION TAG	UNP Q8TDB6
D	589	HIS	-	EXPRESSION TAG	UNP Q8TDB6
D	590	HIS	-	EXPRESSION TAG	UNP Q8TDB6
D	591	HIS	-	EXPRESSION TAG	UNP Q8TDB6
D	592	SER	-	EXPRESSION TAG	UNP Q8TDB6
D	593	SER	-	EXPRESSION TAG	UNP Q8TDB6
D	594	GLY	-	EXPRESSION TAG	UNP Q8TDB6
D	595	LEU	-	EXPRESSION TAG	UNP Q8TDB6
D	596	VAL	-	EXPRESSION TAG	UNP Q8TDB6
D	597	PRO	-	EXPRESSION TAG	UNP Q8TDB6
D	598	ARG	-	EXPRESSION TAG	UNP Q8TDB6
D	599	GLY	-	EXPRESSION TAG	UNP Q8TDB6
D	600	SER	-	EXPRESSION TAG	UNP Q8TDB6

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
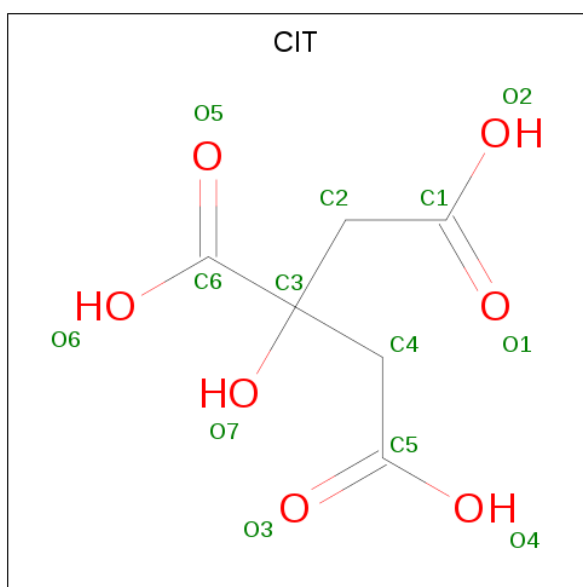
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 12	C 6	O 6	0	0
2	B	1	Total 13	C 6	O 7	0	0
2	C	1	Total 13	C 6	O 7	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

C4

OH O4

O2

O

C3

C1

C2

HO

O1

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	C 4	O 3	0	0
3	B	1	Total 7	C 4	O 3	0	0
3	B	1	Total 7	C 4	O 3	0	0
3	B	1	Total 7	C 4	O 3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1

C2

HO

OH

O1

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total 177	O 177	0	7
5	B	132	Total 136	O 136	0	4
5	C	150	Total 157	O 157	0	7
5	D	155	Total 159	O 159	0	3

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.
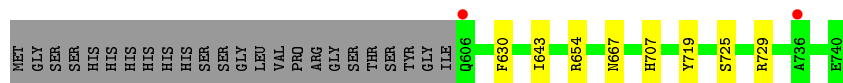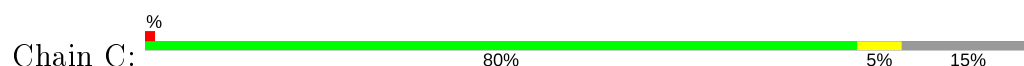
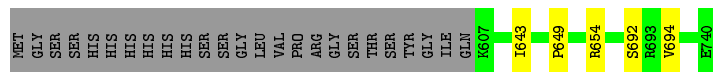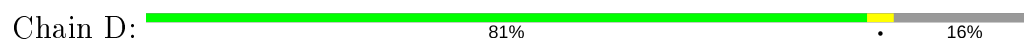- Molecule 1: E3 ubiquitin-protein ligase DTX3L
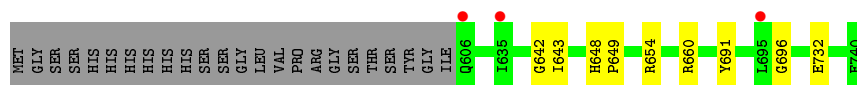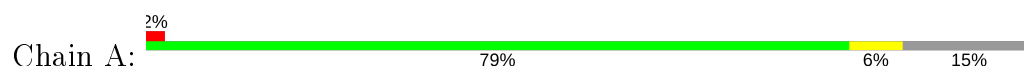
- Molecule 1: E3 ubiquitin-protein ligase DTX3L
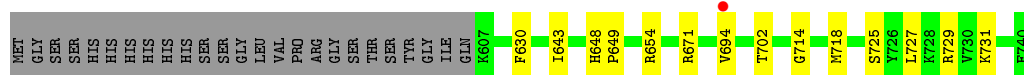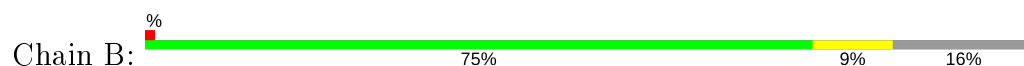
- Molecule 1: E3 ubiquitin-protein ligase DTX3L

- Molecule 1: E3 ubiquitin-protein ligase DTX3L

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.32Å 76.15Å 138.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 29.39 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.70) 99.9 (29.39-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.186 0.176 , 0.195	Depositor DCC
R_{free} test set	2043 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5113	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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, PEG, CIT

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	0.74	1/1125 (0.1%)	0.74	0/1517
1	B	0.71	0/1151	0.73	0/1554
1	C	0.70	0/1139	0.75	0/1535
1	D	0.71	0/1124	0.74	0/1520
All	All	0.71	1/4539 (0.0%)	0.74	0/6126

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	732	GLU	CG-CD	5.07	1.59	1.51

There are no bond angle outliers.

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	1089	0	1083	8	0
1	B	1121	0	1092	12	0
1	C	1109	0	1093	8	0
1	D	1093	0	1058	4	0
2	A	12	0	5	3	0
2	B	13	0	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	5	0	0
3	A	7	0	10	1	0
3	B	21	0	30	4	0
4	D	6	0	8	0	0
5	A	177	0	0	0	0
5	B	136	0	0	0	0
5	C	157	0	0	2	0
5	D	159	0	0	1	0
All	All	5113	0	4389	33	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 4.

The worst 5 of 33 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)
3:B:741:PEG:H41	5:C:1131:HOH:O	1.79	0.82
1:B:643:ILE:CD1	1:B:654:ARG:HG2	2.15	0.76
1:A:643:ILE:HD13	1:A:654:ARG:HG2	1.71	0.70
1:A:660:ARG:HE	2:A:1000:CIT:H22	1.56	0.69
1:A:643:ILE:CD1	1:A:654:ARG:HG2	2.22	0.69

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	137/159 (86%)	136 (99%)	1 (1%)	0	100	100
1	B	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
1	C	138/159 (87%)	138 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	137/159 (86%)	134 (98%)	3 (2%)	0	100 100
All	All	552/636 (87%)	544 (99%)	8 (1%)	0	100 100

There are no Ramachandran outliers to report.

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	118/137 (86%)	118 (100%)	0	100 100
1	B	121/137 (88%)	121 (100%)	0	100 100
1	C	116/137 (85%)	116 (100%)	0	100 100
1	D	115/137 (84%)	115 (100%)	0	100 100
All	All	470/548 (86%)	470 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	CIT	C	1001	-	3,12,12	1.35	1 (33%)	3,17,17	2.40	2 (66%)
3	PEG	B	1002	-	6,6,6	0.46	0	5,5,5	0.29	0
3	PEG	B	1001	-	6,6,6	0.51	0	5,5,5	0.60	0
3	PEG	A	1001	-	6,6,6	0.47	0	5,5,5	0.32	0
2	CIT	B	1000	-	3,12,12	1.28	0	3,17,17	2.99	1 (33%)
3	PEG	B	741	-	6,6,6	0.58	0	5,5,5	0.39	0
2	CIT	A	1000	-	5,11,12	1.98	2 (40%)	4,15,17	5.88	4 (100%)
4	GOL	D	1000	-	5,5,5	0.91	0	5,5,5	0.83	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	CIT	C	1001	-	-	4/6/16/16	-
3	PEG	B	1002	-	-	3/4/4/4	-
3	PEG	B	1001	-	-	3/4/4/4	-
3	PEG	A	1001	-	-	3/4/4/4	-
2	CIT	B	1000	-	-	2/6/16/16	-
3	PEG	B	741	-	-	1/4/4/4	-
2	CIT	A	1000	-	-	7/7/15/16	-
4	GOL	D	1000	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	CIT	O2-C1	-2.44	1.29	1.42
2	A	1000	CIT	C4-C3	2.33	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	CIT	O7-C3	2.14	1.46	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	CIT	C3-C4-C5	8.25	128.19	114.98
2	A	1000	CIT	O2-C1-C2	5.79	126.86	111.39
2	B	1000	CIT	C3-C2-C1	-4.75	107.38	114.98
2	A	1000	CIT	C2-C3-C6	-4.30	103.95	111.52
2	A	1000	CIT	O7-C3-C2	-4.28	96.65	107.15

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1001	CIT	C2-C3-C4-C5
2	C	1001	CIT	O7-C3-C4-C5
2	C	1001	CIT	C6-C3-C4-C5
2	A	1000	CIT	O2-C1-C2-C3
2	A	1000	CIT	C1-C2-C3-O7

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	PEG	1	0
3	A	1001	PEG	1	0
2	B	1000	CIT	3	0
3	B	741	PEG	3	0
2	A	1000	CIT	3	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 (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(Å²)	Q<0.9
1	A	135/159 (84%)	0.08	3 (2%)	62	66	12, 19, 30, 48	0
1	B	134/159 (84%)	-0.06	1 (0%)	87	90	12, 22, 41, 53	0
1	C	135/159 (84%)	-0.02	2 (1%)	73	77	11, 19, 41, 58	0
1	D	134/159 (84%)	-0.25	0	100	100	13, 21, 38, 52	0
All	All	538/636 (84%)	-0.06	6 (1%)	80	83	11, 21, 38, 58	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	606	GLN	3.7
1	A	606	GLN	3.3
1	B	694	VAL	2.7
1	A	695	LEU	2.2
1	C	736	ALA	2.1

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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	CIT	C	1001	13/13	0.65	0.26	48,55,56,58	0
3	PEG	B	1002	7/7	0.69	0.35	67,69,71,72	0
4	GOL	D	1000	6/6	0.69	0.19	24,31,32,38	0
3	PEG	B	741	7/7	0.72	0.38	53,56,56,56	0
2	CIT	B	1000	13/13	0.72	0.22	50,57,62,63	0
3	PEG	A	1001	7/7	0.75	0.39	50,57,60,60	0
2	CIT	A	1000	12/13	0.83	0.16	21,35,45,46	0
3	PEG	B	1001	7/7	0.83	0.25	47,48,51,53	0

6.5 Other polymers (i)

There are no such residues in this entry.