



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:09 AM UTC

PDB ID : 3PG6 / pdb_00003pg6
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

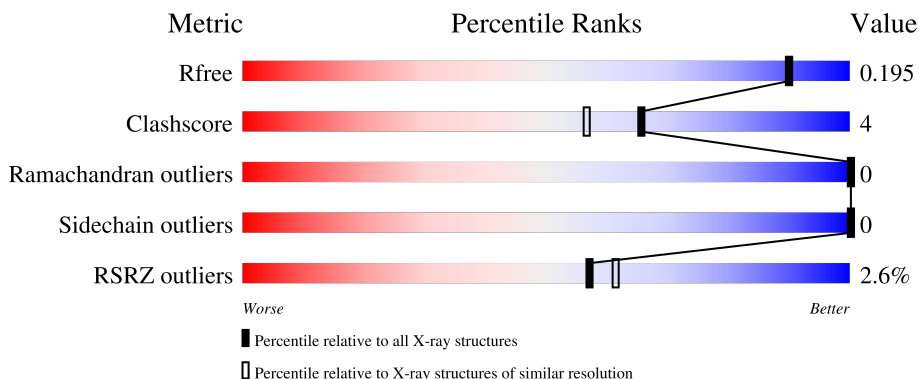
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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 $\leq 5\%$. 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	159	 3% 79% 6% 15%
1	B	159	 3% 75% 9% 16%
1	C	159	 3% 80% 5% 15%
1	D	159	 81% 16% 3%

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	CIT	A	1000	-	X	-	-

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

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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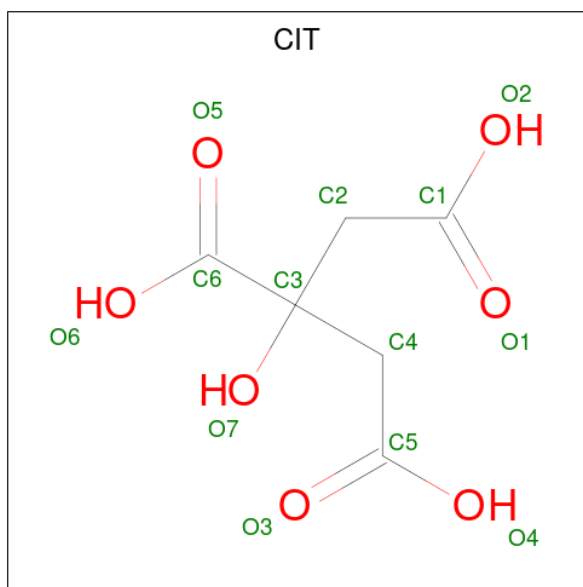
Chain	Residue	Modelled	Actual	Comment	Reference
B	584	SER	-	expression tag	UNP Q8TDB6
B	585	SER	-	expression tag	UNP Q8TDB6
B	586	HIS	-	expression tag	UNP Q8TDB6
B	587	HIS	-	expression tag	UNP Q8TDB6
B	588	HIS	-	expression tag	UNP Q8TDB6
B	589	HIS	-	expression tag	UNP Q8TDB6
B	590	HIS	-	expression tag	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 (CCD ID: CIT) (formula: $C_6H_8O_7$).



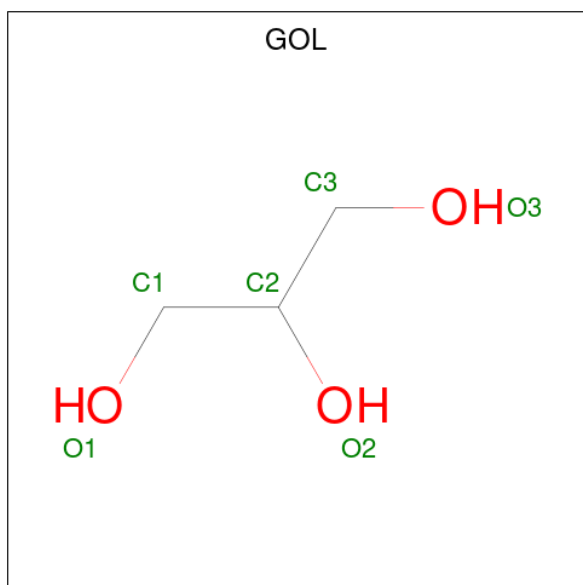
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

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

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 30.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.70) 99.9 (30.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.70Å)	Xtrriage
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	Xtrriage
Anisotropy	0.003	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for k,h,-l	Xtrriage
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

Xtrriage'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.*

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: CIT, GOL, PEG

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	0.84	0/1125	0.88	1/1517 (0.1%)
1	B	0.78	0/1151	0.83	0/1554
1	C	0.81	0/1139	0.84	0/1535
1	D	0.77	0/1124	0.80	0/1520
All	All	0.80	0/4539	0.84	1/6126 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	693	ARG	N-CA-C	6.10	117.60	111.07

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	1089	0	1083	8	0
1	B	1121	0	1092	13	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	4	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	34	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.

All (34) 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
1:B:718:MET:HG3	3:B:741:PEG:H42	1.80	0.63
1:B:643:ILE:HD13	1:B:654:ARG:HG2	1.80	0.62
1:B:725:SER:OG	1:B:729[A]:ARG:NH2	2.33	0.62
1:D:643:ILE:HG12	1:D:654:ARG:HG2	1.85	0.59
1:A:642:GLY:HA2	3:A:1001:PEG:H31	1.83	0.59
1:B:714:GLY:HA2	3:B:741:PEG:H11	1.87	0.57
1:D:649:PRO:HG2	5:D:1034:HOH:O	2.04	0.57
1:A:660:ARG:HE	2:A:1000:CIT:C2	2.17	0.56
1:C:729[B]:ARG:HG3	5:C:1111:HOH:O	2.07	0.55
1:C:725:SER:HB2	1:C:729[B]:ARG:HH11	1.72	0.54
1:A:648:HIS:HB3	1:A:649:PRO:HD2	1.90	0.54
2:B:1000:CIT:C6	2:B:1000:CIT:O2	2.58	0.51
1:B:694:VAL:HG23	2:B:1000:CIT:O7	2.10	0.51
1:B:630:PHE:CE1	3:B:1001:PEG:H22	2.46	0.50
1:C:643[B]:ILE:HD13	1:C:654:ARG:HG2	1.94	0.49
1:C:725:SER:HB2	1:C:729[B]:ARG:NH1	2.27	0.49
1:B:702[A]:THR:HG1	2:B:1000:CIT:C5	2.26	0.47
1:A:691:TYR:CZ	1:A:696:GLY:HA2	2.50	0.47
1:B:702[A]:THR:OG1	2:B:1000:CIT:O3	2.30	0.47
1:C:643[B]:ILE:CD1	1:C:654:ARG:HG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LEU:O	1:B:731:LYS:HG3	2.17	0.45
1:D:692:SER:OG	1:D:694[A]:VAL:HG12	2.18	0.43
1:B:643:ILE:HD11	1:B:654:ARG:NH1	2.33	0.42
1:B:671:ARG:HD2	1:D:643:ILE:HG21	2.00	0.42
1:A:660:ARG:HH21	2:A:1000:CIT:H22	1.86	0.41
1:C:630:PHE:CG	1:C:667:ASN:HB3	2.55	0.41
1:B:648:HIS:HB3	1:B:649:PRO:HD2	2.02	0.40
1:C:725:SER:CB	1:C:729[B]:ARG:HH11	2.34	0.40
1:C:707:HIS:HE1	1:C:719:TYR:HD2	1.68	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	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
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.

Sometimes 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 oligosaccharides 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	$\# Z > 2$
3	PEG	A	1001	-	6,6,6	0.48	0	5,5,5	0.32	0
3	PEG	B	1002	-	6,6,6	0.46	0	5,5,5	0.29	0
4	GOL	D	1000	-	5,5,5	0.93	0	5,5,5	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	A	1000	-	11,11,12	1.87	4 (36%)	12,15,17	4.19	7 (58%)
3	PEG	B	741	-	6,6,6	0.59	0	5,5,5	0.39	0
3	PEG	B	1001	-	6,6,6	0.52	0	5,5,5	0.59	0
2	CIT	B	1000	-	12,12,12	1.05	0	17,17,17	1.82	6 (35%)
2	CIT	C	1001	-	12,12,12	1.27	0	17,17,17	1.82	7 (41%)

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	PEG	A	1001	-	-	3/4/4/4	-
3	PEG	B	1002	-	-	3/4/4/4	-
4	GOL	D	1000	-	-	0/4/4/4	-
2	CIT	A	1000	-	-	11/15/15/16	-
3	PEG	B	741	-	-	1/4/4/4	-
3	PEG	B	1001	-	-	3/4/4/4	-
2	CIT	B	1000	-	-	2/16/16/16	-
2	CIT	C	1001	-	-	3/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	CIT	C4-C3	3.42	1.58	1.54
2	A	1000	CIT	O3-C5	2.68	1.30	1.22
2	A	1000	CIT	O2-C1	-2.47	1.29	1.42
2	A	1000	CIT	C4-C5	2.02	1.56	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	CIT	O7-C3-C2	-7.65	96.65	108.88
2	A	1000	CIT	O7-C3-C6	5.95	117.40	108.96
2	A	1000	CIT	O2-C1-C2	5.53	126.86	111.33
2	A	1000	CIT	C3-C4-C5	5.22	128.19	113.92
2	A	1000	CIT	O6-C6-C3	5.07	122.87	113.14
2	A	1000	CIT	O4-C5-O3	-3.97	113.13	123.33
2	C	1001	CIT	O6-C6-C3	3.93	120.68	113.14
2	B	1000	CIT	O7-C3-C6	-3.55	103.92	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	CIT	O6-C6-C3	2.74	118.40	113.14
2	C	1001	CIT	O2-C1-C2	2.50	122.26	114.35
2	A	1000	CIT	O5-C6-C3	-2.44	117.36	122.09
2	B	1000	CIT	C3-C2-C1	-2.39	107.38	113.92
2	B	1000	CIT	O2-C1-C2	2.33	121.74	114.35
2	B	1000	CIT	O4-C5-O3	-2.32	117.37	123.33
2	C	1001	CIT	O2-C1-O1	-2.25	117.54	123.33
2	C	1001	CIT	O4-C5-O3	-2.20	117.67	123.33
2	C	1001	CIT	O6-C6-O5	-2.18	116.87	123.86
2	B	1000	CIT	C4-C3-C6	2.09	114.66	110.03
2	C	1001	CIT	C3-C4-C5	2.04	119.50	113.92
2	C	1001	CIT	C3-C2-C1	2.01	119.41	113.92

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	CIT	O2-C1-C2-C3
2	A	1000	CIT	C1-C2-C3-O7
2	A	1000	CIT	C1-C2-C3-C4
2	A	1000	CIT	C1-C2-C3-C6
2	A	1000	CIT	C2-C3-C4-C5
2	A	1000	CIT	O7-C3-C4-C5
2	C	1001	CIT	O7-C3-C4-C5
2	C	1001	CIT	C6-C3-C4-C5
2	A	1000	CIT	C6-C3-C4-C5
2	C	1001	CIT	C2-C3-C4-C5
3	B	1002	PEG	O1-C1-C2-O2
3	B	1002	PEG	O2-C3-C4-O4
3	A	1001	PEG	O1-C1-C2-O2
3	B	1001	PEG	O1-C1-C2-O2
3	B	1001	PEG	C1-C2-O2-C3
3	B	1001	PEG	C4-C3-O2-C2
3	A	1001	PEG	C1-C2-O2-C3
3	A	1001	PEG	O2-C3-C4-O4
2	A	1000	CIT	C2-C3-C6-O6
2	A	1000	CIT	C4-C3-C6-O6
3	B	741	PEG	O2-C3-C4-O4
2	B	1000	CIT	O7-C3-C4-C5
3	B	1002	PEG	C4-C3-O2-C2
2	A	1000	CIT	C2-C3-C6-O5
2	B	1000	CIT	C4-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
2	A	1000	CIT	C4-C3-C6-O5

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	PEG	1	0
2	A	1000	CIT	3	0
3	B	741	PEG	3	0
3	B	1001	PEG	1	0
2	B	1000	CIT	4	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(Å ²)	Q<0.9
1	A	135/159 (84%)	-0.24	4 (2%) 52 56	7, 19, 30, 48	3 (2%)
1	B	134/159 (84%)	-0.06	5 (3%) 45 49	7, 22, 41, 53	7 (5%)
1	C	135/159 (84%)	-0.13	5 (3%) 45 49	7, 19, 41, 58	5 (3%)
1	D	134/159 (84%)	-0.16	0 100 100	10, 21, 38, 52	5 (3%)
All	All	538/636 (84%)	-0.15	14 (2%) 57 61	7, 20, 38, 58	20 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	694	VAL	5.0
1	A	695	LEU	3.5
1	A	694	VAL	3.5
1	C	694	VAL	3.4
1	C	606	GLN	3.1
1	C	697	VAL	3.1
1	A	606	GLN	2.8
1	C	695	LEU	2.7
1	B	705	ASP	2.5
1	A	696	GLY	2.5
1	C	696	GLY	2.3
1	B	695	LEU	2.3
1	B	729[A]	ARG	2.2
1	B	739	ILE	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 oligosaccharides 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(\AA^2)	Q<0.9
2	CIT	C	1001	13/13	0.67	0.18	48,55,56,58	0
3	PEG	B	741	7/7	0.70	0.22	53,56,56,56	0
3	PEG	B	1002	7/7	0.73	0.21	67,69,71,72	0
3	PEG	B	1001	7/7	0.74	0.22	47,48,51,53	0
2	CIT	B	1000	13/13	0.74	0.18	50,57,62,63	0
4	GOL	D	1000	6/6	0.74	0.16	24,31,32,38	0
3	PEG	A	1001	7/7	0.81	0.18	50,57,60,60	0
2	CIT	A	1000	12/13	0.82	0.15	21,35,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.