Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:27 AM GMT

PDB ID	:	2H77
Title	:	Crystal structure of human TR alpha bound T3 in monoclinic space group
Authors	:	Nascimento, A.S.; Dias, S.M.G.; Nunes, F.M.; Aparicio, R.; Bleicher, L.; Ambrosio, A.L.B.; Figueira, A.C.M.; Santos, M.A.M.; Neto, M.O.; Fischer, H.; Togashi, H.F.M; Craievich, A.F.; Garrat, R.C.; Baxter, J.D.; Webb, P.; Polikarpov, I.
Deposited on	:	2006-06-01
Resolution	:	2.33 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 (i) symbol.

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

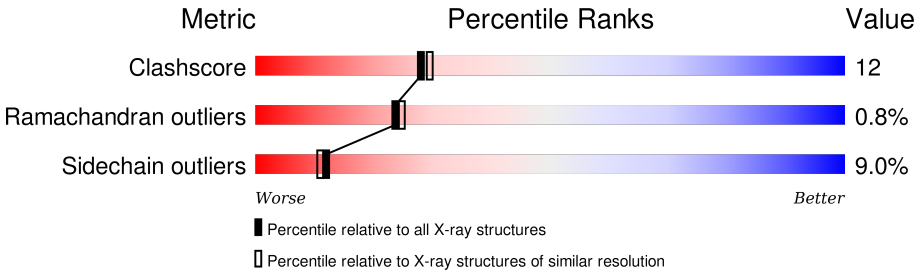
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.33 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))
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	61% 28% 6% • 5%

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
1	CAS	A	334	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2140 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.

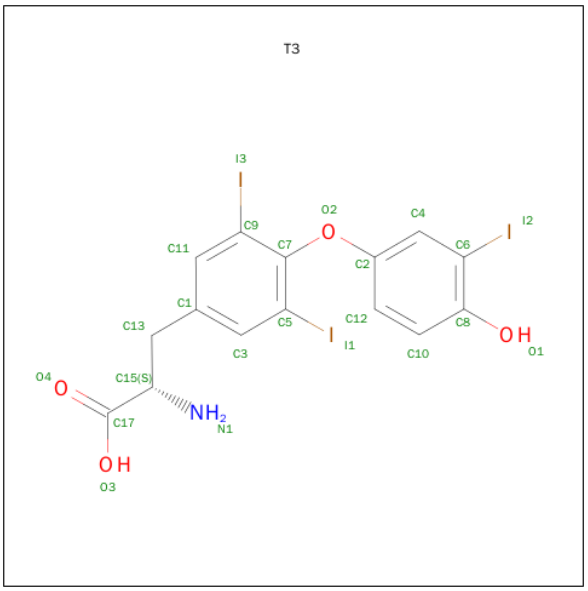
- Molecule 1 is a protein called THRA protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	255	Total	As	C	N	O	S	0	13	0
			2047	4	1305	348	375	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ALA	-	CLONING ARTIFACT	UNP Q6FH41
A	143	ARG	-	CLONING ARTIFACT	UNP Q6FH41
A	144	GLY	-	CLONING ARTIFACT	UNP Q6FH41
A	145	SER	-	CLONING ARTIFACT	UNP Q6FH41
A	146	HIS	-	CLONING ARTIFACT	UNP Q6FH41
A	147	MET	-	CLONING ARTIFACT	UNP Q6FH41
A	334	CAS	CYS	MODIFIED RESIDUE	UNP Q6FH41
A	380	CAS	CYS	MODIFIED RESIDUE	UNP Q6FH41
A	388	CAS	MET	ENGINEERED	UNP Q6FH41
A	392	CAS	CYS	MODIFIED RESIDUE	UNP Q6FH41

- Molecule 2 is 3,5,3'TRIIODOTHYRONINE (three-letter code: T3) (formula: $C_{15}H_{12}I_3NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	0	0
			23	15	3	1	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		

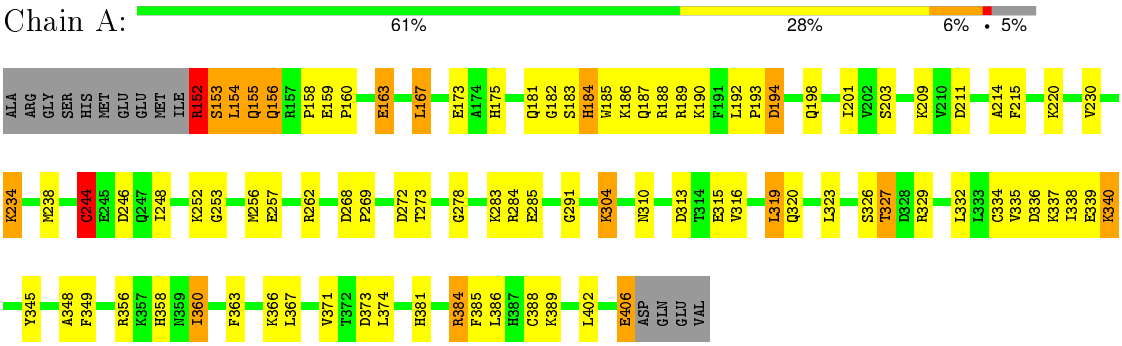
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: THRA protein

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.57Å 80.63Å 62.61Å 90.00° 121.09° 90.00°	Depositor
Resolution (Å)	32.22 – 2.33	Depositor
% Data completeness (in resolution range)	85.9 (32.22-2.33)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2140	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, T3

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	1.25	8/2055 (0.4%)	1.10	9/2772 (0.3%)

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	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	GLU	CG-CD	8.09	1.64	1.51
1	A	173	GLU	CG-CD	6.24	1.61	1.51
1	A	345	TYR	CD1-CE1	6.12	1.48	1.39
1	A	348	ALA	CA-CB	5.96	1.65	1.52
1	A	214	ALA	CA-CB	5.73	1.64	1.52
1	A	244	CYS	CB-SG	-5.64	1.72	1.81
1	A	285	GLU	CG-CD	5.59	1.60	1.51
1	A	173	GLU	CD-OE1	5.23	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	ASP	CB-CG-OD2	9.14	126.53	118.30
1	A	384	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	373	ASP	CB-CG-OD1	7.47	125.02	118.30
1	A	167	LEU	CA-CB-CG	7.14	131.73	115.30
1	A	323	LEU	CB-CG-CD1	-6.26	100.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	384	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	313	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	167	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	A	304	LYS	CD-CE-NZ	5.06	123.33	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Peptide
1	A	153	SER	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	2047	0	2010	48	50
2	A	23	0	8	1	0
3	A	70	0	0	3	3
All	All	2140	0	2018	48	50

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 12.

All (48) 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:163:GLU:HG3	3:A:435:HOH:O	1.63	0.98
1:A:310:ASN:OD1	3:A:472:HOH:O	1.89	0.91
1:A:272:ASP:OD1	1:A:284[B]:ARG:NH1	2.12	0.83
1:A:175:HIS:HD2	1:A:262:ARG:HH21	1.25	0.80
1:A:153:SER:H	1:A:159:GLU:HB2	1.56	0.71
1:A:385:PHE:CE2	1:A:389:LYS:HD3	2.28	0.69
1:A:381:HIS:HE1	2:A:1:T3:O1	1.79	0.66
1:A:215:PHE:CD1	1:A:388:CAS:CE1	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:OG	1:A:209:LYS:HE2	1.97	0.65
1:A:215:PHE:CE1	1:A:388:CAS:CE1	2.80	0.64
1:A:155:GLN:O	1:A:156:GLN:HG2	1.98	0.62
1:A:402:LEU:O	1:A:406:GLU:HB3	2.00	0.62
1:A:334:CAS:CE2	3:A:429:HOH:O	2.48	0.61
1:A:316:VAL:O	1:A:320:GLN:HG3	2.04	0.57
1:A:360:ILE:HD11	1:A:366:LYS:HD3	1.87	0.56
1:A:291:GLY:O	1:A:384:ARG:HD3	2.06	0.54
1:A:315:GLU:OE2	1:A:358:HIS:HE1	1.89	0.54
1:A:315:GLU:O	1:A:319:LEU:HB2	2.10	0.52
1:A:167:LEU:HD11	1:A:238:MET:HE1	1.92	0.52
1:A:175:HIS:CD2	1:A:262:ARG:HH21	2.17	0.52
1:A:248:ILE:O	1:A:252:LYS:HG3	2.10	0.51
1:A:153:SER:HA	1:A:158:PRO:HA	1.93	0.51
1:A:152:ARG:HG3	1:A:159:GLU:HB2	1.92	0.51
1:A:273:THR:HG22	1:A:283:LYS:HD2	1.94	0.50
1:A:244:CYS:O	1:A:248:ILE:HG13	2.12	0.49
1:A:256:MET:HG2	1:A:381:HIS:CG	2.47	0.49
1:A:230:VAL:HG12	1:A:234:LYS:HD3	1.96	0.47
1:A:194:ASP:O	1:A:198:GLN:NE2	2.40	0.47
1:A:363:PHE:CE2	1:A:367:LEU:HD22	2.50	0.47
1:A:152:ARG:HD2	1:A:160:PRO:O	2.14	0.46
1:A:192:LEU:HD12	1:A:193:PRO:HD2	1.97	0.46
1:A:167:LEU:HD11	1:A:238:MET:CE	2.46	0.46
1:A:257[A]:GLU:HG2	1:A:374:LEU:O	2.16	0.45
1:A:319:LEU:CD1	1:A:371:VAL:HG22	2.47	0.44
1:A:284[B]:ARG:NH2	1:A:304:LYS:NZ	2.66	0.44
1:A:385:PHE:HE2	1:A:389:LYS:HD3	1.79	0.43
1:A:215:PHE:HE1	1:A:388:CAS:CE1	2.29	0.43
1:A:152:ARG:HG3	1:A:153:SER:N	2.34	0.43
1:A:152:ARG:N	1:A:154:LEU:HB2	2.33	0.43
1:A:253:GLY:O	1:A:329:ARG:NH2	2.53	0.42
1:A:268:ASP:HA	1:A:269:PRO:HD3	1.91	0.42
1:A:272:ASP:CG	1:A:284[B]:ARG:HH11	2.23	0.42
1:A:152:ARG:HA	1:A:159:GLU:HG3	2.02	0.42
1:A:310:ASN:O	1:A:356:ARG:NH2	2.53	0.41
1:A:327:THR:HG23	1:A:327:THR:O	2.21	0.41
1:A:152:ARG:HG3	1:A:153:SER:H	1.86	0.41
1:A:185:TRP:O	1:A:189:ARG:HG2	2.21	0.41

All (50) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:N	1:A:334:CAS:CA[4_545]	0.38	1.82
1:A:188:ARG:CG	1:A:335:VAL:C[4_545]	0.95	1.25
1:A:188:ARG:NE	1:A:335:VAL:CG1[4_545]	0.96	1.24
1:A:188:ARG:CG	1:A:335:VAL:O[4_545]	1.03	1.17
1:A:187:GLN:NE2	1:A:246:ASP:OD2[4_545]	1.15	1.05
1:A:184:HIS:CB	1:A:335:VAL:CG2[4_545]	1.22	0.98
1:A:188:ARG:CB	1:A:335:VAL:C[4_545]	1.25	0.95
1:A:183:SER:O	1:A:332:LEU:O[4_545]	1.39	0.81
1:A:188:ARG:CD	1:A:335:VAL:CG1[4_545]	1.39	0.81
1:A:184:HIS:O	1:A:335:VAL:N[4_545]	1.42	0.78
1:A:184:HIS:O	1:A:335:VAL:CB[4_545]	1.49	0.71
1:A:278:GLY:O	1:A:336[A]:ASP:OD2[4_545]	1.49	0.71
1:A:187:GLN:CD	1:A:246:ASP:OD2[4_545]	1.58	0.62
1:A:184:HIS:O	1:A:335:VAL:CA[4_545]	1.63	0.57
1:A:188:ARG:C	1:A:337:LYS:N[4_545]	1.64	0.56
1:A:187:GLN:O	1:A:338:ILE:N[4_545]	1.74	0.46
1:A:189:ARG:N	3:A:429:HOH:O[4_545]	1.74	0.46
1:A:188:ARG:CA	1:A:337:LYS:N[4_545]	1.79	0.41
1:A:184:HIS:CA	1:A:335:VAL:CG2[4_545]	1.79	0.41
1:A:188:ARG:CA	1:A:335:VAL:C[4_545]	1.83	0.37
1:A:187:GLN:CA	1:A:334:CAS:CA[4_545]	1.84	0.36
1:A:188:ARG:N	1:A:334:CAS:C[4_545]	1.84	0.36
1:A:181:GLN:NE2	1:A:336[A]:ASP:OD1[4_545]	1.85	0.35
1:A:184:HIS:O	1:A:335:VAL:CG2[4_545]	1.86	0.34
1:A:183:SER:C	1:A:332:LEU:O[4_545]	1.87	0.33
1:A:189:ARG:NE	1:A:334:CAS:CE2[4_545]	1.88	0.32
1:A:184:HIS:CA	1:A:332:LEU:O[4_545]	1.90	0.30
1:A:188:ARG:CG	1:A:335:VAL:CA[4_545]	1.91	0.29
1:A:187:GLN:C	1:A:334:CAS:C[4_545]	1.92	0.28
1:A:188:ARG:CB	1:A:335:VAL:O[4_545]	1.93	0.27
1:A:187:GLN:NE2	1:A:246:ASP:CG[4_545]	1.94	0.26
1:A:184:HIS:C	1:A:335:VAL:CG2[4_545]	1.95	0.25
1:A:187:GLN:CG	1:A:246:ASP:OD2[4_545]	1.98	0.22
1:A:185:TRP:O	3:A:429:HOH:O[4_545]	1.98	0.22
1:A:187:GLN:O	1:A:337:LYS:CA[4_545]	2.00	0.20
1:A:187:GLN:CB	1:A:338:ILE:CD1[4_545]	2.03	0.17
1:A:184:HIS:N	1:A:332:LEU:O[4_545]	2.04	0.16
1:A:187:GLN:O	1:A:334:CAS:O[4_545]	2.05	0.15
1:A:188:ARG:N	1:A:335:VAL:C[4_545]	2.06	0.14
1:A:188:ARG:CZ	1:A:335:VAL:CG1[4_545]	2.06	0.14
1:A:187:GLN:O	1:A:337:LYS:N[4_545]	2.07	0.13
1:A:278:GLY:C	1:A:336[A]:ASP:OD2[4_545]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:N	1:A:334:CAS:O[4_545]	2.08	0.12
1:A:187:GLN:O	1:A:337:LYS:CB[4_545]	2.08	0.12
1:A:187:GLN:NE2	1:A:334:CAS:N[4_545]	2.10	0.10
1:A:187:GLN:CD	1:A:334:CAS:N[4_545]	2.11	0.09
1:A:187:GLN:O	1:A:337:LYS:C[4_545]	2.13	0.07
1:A:189:ARG:CG	3:A:429:HOH:O[4_545]	2.15	0.05
1:A:188:ARG:N	1:A:335:VAL:N[4_545]	2.15	0.05
1:A:188:ARG:O	1:A:337:LYS:N[4_545]	2.17	0.03

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	250/269 (93%)	241 (96%)	7 (3%)	2 (1%)	24 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	182	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	224/235 (95%)	204 (91%)	20 (9%)	12 11

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	154	LEU
1	A	155	GLN
1	A	184	HIS
1	A	186	LYS
1	A	190	LYS
1	A	194	ASP
1	A	201	ILE
1	A	220	LYS
1	A	234	LYS
1	A	244	CYS
1	A	319	LEU
1	A	326	SER
1	A	327	THR
1	A	339	GLU
1	A	340	LYS
1	A	349	PHE
1	A	360	ILE
1	A	386	LEU
1	A	406	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	A	310	ASN
1	A	358	HIS
1	A	381	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CAS	A	334	1	5,8,9	1.45	1 (20%)	2,9,11	1.62	1 (50%)
1	CAS	A	380	1	5,8,9	1.30	1 (20%)	2,9,11	1.25	0
1	CAS	A	388	1	5,8,9	1.35	0	2,9,11	2.13	2 (100%)
1	CAS	A	392[A]	-	5,8,9	0.77	0	2,9,11	2.45	2 (100%)

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
1	CAS	A	334	1	-	0/0/7/9	0/0/0/0
1	CAS	A	380	1	-	0/0/7/9	0/0/0/0
1	CAS	A	388	1	-	0/0/7/9	0/0/0/0
1	CAS	A	392[A]	-	-	0/0/7/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	CAS	AS-CE2	2.16	2.01	1.96
1	A	334	CAS	AS-CE1	2.29	2.02	1.96

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	392[A]	CAS	CA-CB-SG	-2.56	105.07	114.16
1	A	392[A]	CAS	O-C-CA	-2.34	119.39	125.49
1	A	388	CAS	CA-CB-SG	-2.15	106.50	114.16
1	A	388	CAS	O-C-CA	-2.10	120.02	125.49
1	A	334	CAS	O-C-CA	-2.05	120.16	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	334	CAS	1	9
1	A	388	CAS	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	T3	A	1	-	21,24,24	3.74	9 (42%)	27,34,34	8.41	16 (59%)

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	T3	A	1	-	-	0/8/12/12	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	T3	C4-C2	-8.56	1.23	1.38
2	A	1	T3	C3-C1	-7.32	1.26	1.39
2	A	1	T3	C12-C10	-6.83	1.26	1.38
2	A	1	T3	C10-C8	-5.67	1.29	1.39
2	A	1	T3	C3-C5	-5.33	1.26	1.39
2	A	1	T3	C4-C6	-5.16	1.26	1.39
2	A	1	T3	C11-C9	2.52	1.45	1.39
2	A	1	T3	O2-C2	2.73	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	T3	C9-I3	3.73	2.19	2.10

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	T3	C10-C8-C6	-19.07	101.96	119.37
2	A	1	T3	C10-C12-C2	-11.12	105.74	119.74
2	A	1	T3	C11-C1-C3	-9.82	104.50	118.96
2	A	1	T3	C12-C2-C4	-9.08	107.80	120.56
2	A	1	T3	C3-C5-C7	-6.09	108.24	121.67
2	A	1	T3	O2-C2-C4	2.18	125.64	119.04
2	A	1	T3	C7-C9-I3	2.71	124.55	119.31
2	A	1	T3	C13-C1-C11	3.12	126.38	120.36
2	A	1	T3	O1-C8-C6	4.03	125.47	119.16
2	A	1	T3	C13-C1-C3	4.52	129.07	120.36
2	A	1	T3	O1-C8-C10	4.78	132.48	119.35
2	A	1	T3	C3-C5-I1	5.40	128.84	118.60
2	A	1	T3	C4-C6-I2	5.93	129.84	118.60
2	A	1	T3	C2-C4-C6	9.40	145.68	118.96
2	A	1	T3	C1-C3-C5	13.35	149.35	120.36
2	A	1	T3	C12-C10-C8	27.86	149.08	120.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	T3	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.