



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:12 AM GMT

PDB ID : 2PUV
Title : The crystal structure of isomerase domain of glucosamine-6-phosphate synthase from *Candida albicans*
Authors : Raczynska, J.; Olchow, J.; Milewski, S.; Rypniewski, W.
Deposited on : 2007-05-09
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

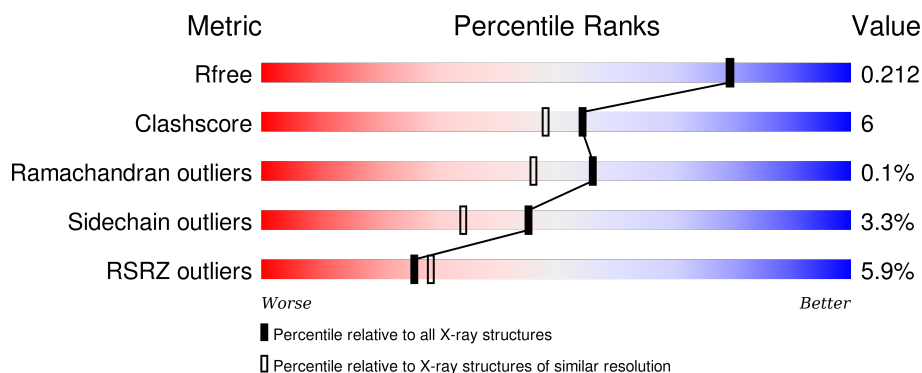
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	367	<div> <div>5%</div> <div>78% 13% 8%</div> </div>
1	B	367	<div> <div>5%</div> <div>83% 13%</div> </div>
1	C	367	<div> <div>8%</div> <div>80% 13% 5%</div> </div>
1	D	367	<div> <div>4%</div> <div>79% 13% 7%</div> </div>

2 Entry composition [i](#)

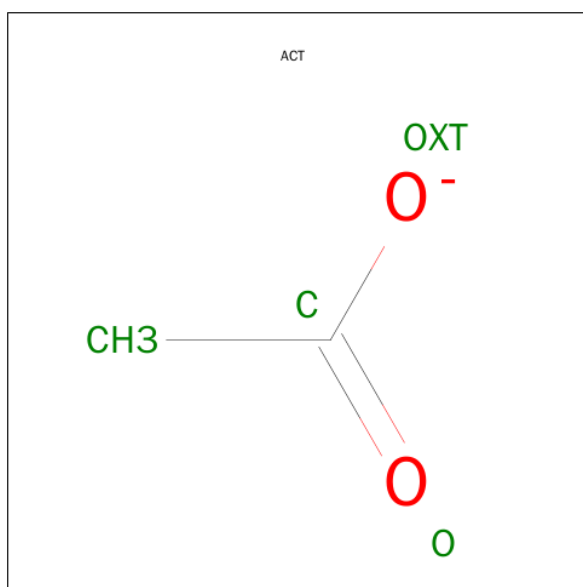
There are 6 unique types of molecules in this entry. The entry contains 11724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	2	0
			2627	1659	454	497	17			
1	B	352	Total	C	N	O	S	0	2	0
			2739	1730	473	519	17			
1	C	348	Total	C	N	O	S	0	2	0
			2707	1710	467	512	18			
1	D	340	Total	C	N	O	S	0	4	0
			2650	1672	460	501	17			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

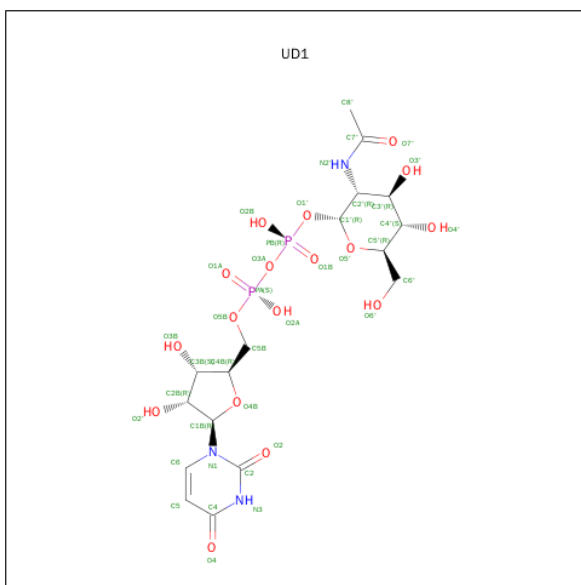


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

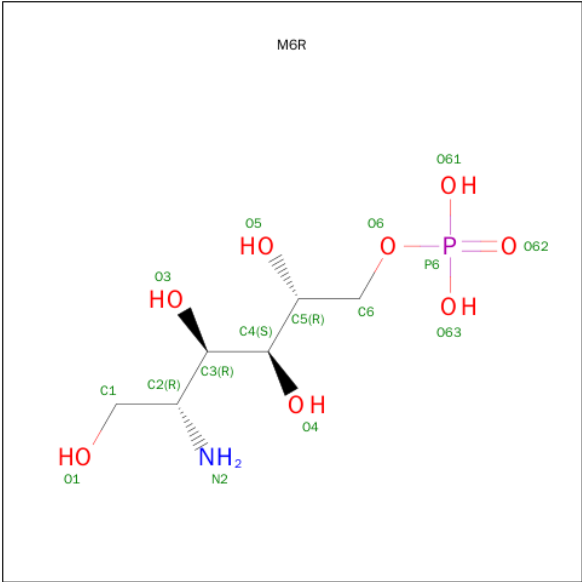
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 5 is 5-AMINO-5-DEOXY-1-O-PHOSPHONO-D-MANNITOL (three-letter code: M6R) (formula: C₆H₁₆NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
5	B	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
5	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
5	D	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

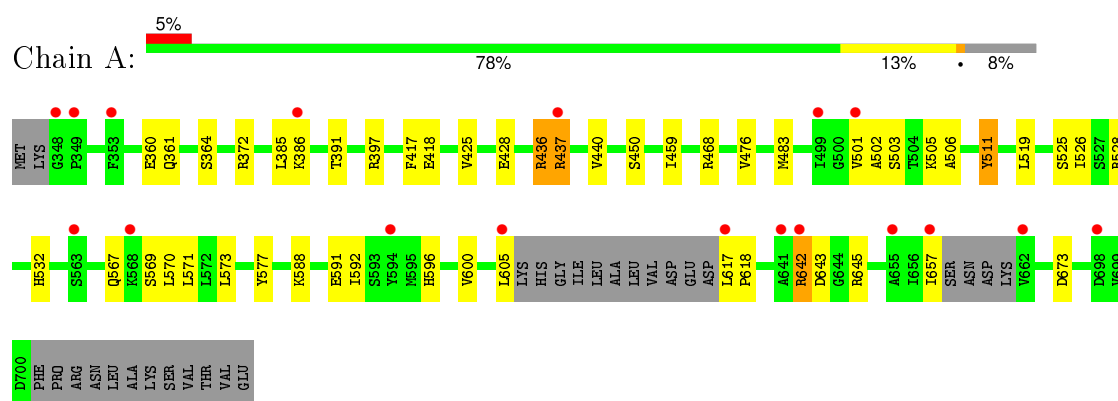
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	177	Total	O	0	0
			177	177		
6	B	195	Total	O	0	0
			195	195		
6	C	190	Total	O	0	0
			190	190		
6	D	207	Total	O	0	0
			207	207		

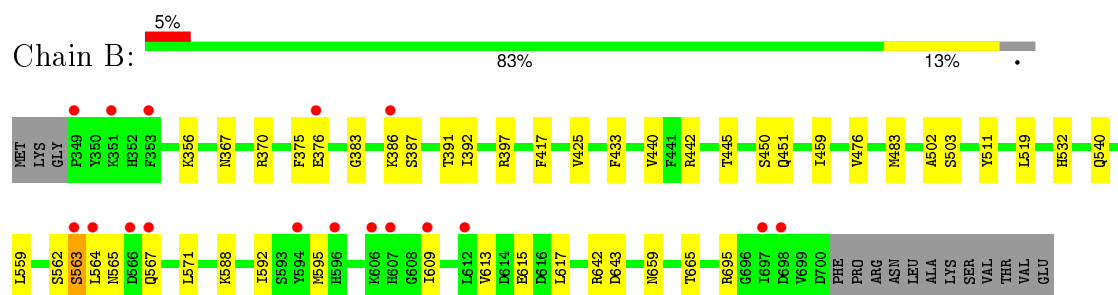
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

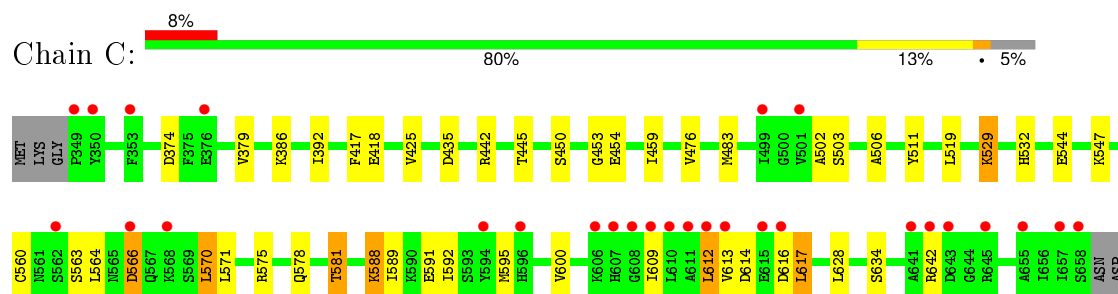
- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)

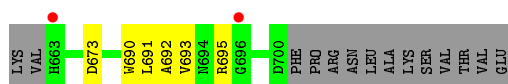


- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)

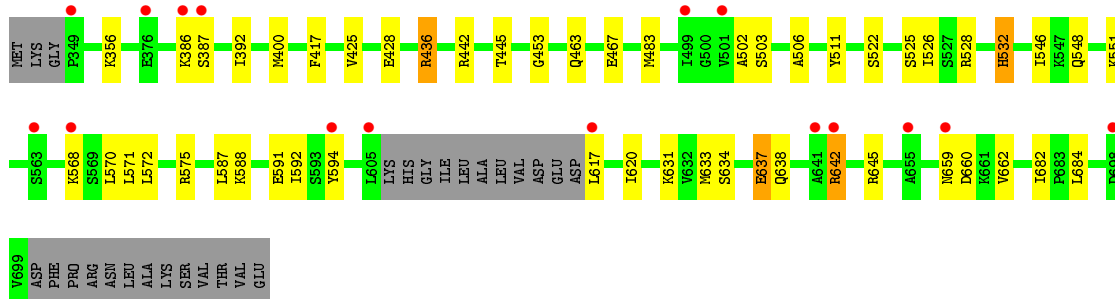
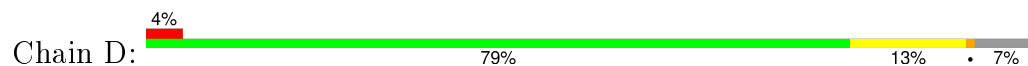


- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)





- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.12Å 118.17Å 100.14Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	19.93 – 1.90 19.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.93-1.90) 99.8 (19.93-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.171 , 0.212 0.172 , 0.212	Depositor DCC
R_{free} test set	2424 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.1	EDS
Estimated twinning fraction	0.058 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 120507 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11724	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, M6R, UD1, ACT

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	2/2672 (0.1%)	0.85	5/3609 (0.1%)
1	B	0.78	0/2787	0.77	0/3767
1	C	0.80	1/2754 (0.0%)	0.82	5/3720 (0.1%)
1	D	0.80	0/2701	0.84	2/3649 (0.1%)
All	All	0.81	3/10914 (0.0%)	0.82	12/14745 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	GLU	CD-OE1	5.91	1.32	1.25
1	C	418	GLU	CD-OE1	5.87	1.32	1.25
1	A	577	TYR	CD1-CE1	5.50	1.47	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	436	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	C	575	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	575	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	436	ARG	NE-CZ-NH1	6.09	123.34	120.30

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	2627	0	2673	40	0
1	B	2739	0	2796	24	0
1	C	2707	0	2761	37	0
1	D	2650	0	2707	43	0
2	A	4	0	3	0	0
2	C	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	39	0	25	0	0
4	B	39	0	25	0	0
4	C	39	0	25	0	0
4	D	39	0	25	1	0
5	A	16	0	14	1	0
5	B	16	0	14	1	0
5	C	16	0	14	2	0
5	D	16	0	14	1	0
6	A	177	0	0	3	0
6	B	195	0	0	4	0
6	C	190	0	0	3	0
6	D	207	0	0	5	0
All	All	11724	0	11099	140	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 6.

The worst 5 of 140 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:D:400:MET:HE2	1:D:425:VAL:HG11	1.19	1.07
1:D:400:MET:HE2	1:D:425:VAL:CG1	1.92	0.99
1:C:609:ILE:HA	6:C:5742:HOH:O	1.64	0.97
1:D:400:MET:CE	1:D:425:VAL:CG1	2.42	0.96
1:D:502:ALA:HB2	1:D:592:ILE:HD11	1.48	0.96

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	334/367 (91%)	330 (99%)	4 (1%)	0	100	100
1	B	352/367 (96%)	344 (98%)	7 (2%)	1 (0%)	46	35
1	C	346/367 (94%)	340 (98%)	5 (1%)	1 (0%)	46	35
1	D	340/367 (93%)	338 (99%)	2 (1%)	0	100	100
All	All	1372/1468 (94%)	1352 (98%)	18 (1%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	386	LYS
1	B	563	SER

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	294/319 (92%)	285 (97%)	9 (3%)	47	37
1	B	308/319 (97%)	297 (96%)	11 (4%)	42	30
1	C	304/319 (95%)	291 (96%)	13 (4%)	35	23
1	D	298/319 (93%)	292 (98%)	6 (2%)	63	57
All	All	1204/1276 (94%)	1165 (97%)	39 (3%)	45	35

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	567	GLN
1	C	529	LYS
1	D	568	LYS
1	B	615	GLU
1	B	643	ASP

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	561	ASN
1	D	532	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](#)

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](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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
4	UD1	A	5002	3	32,41,41	0.76	1 (3%)	46,62,62	1.50	4 (8%)
5	M6R	A	5003	-	15,15,15	1.07	1 (6%)	14,21,21	1.02	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	713	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
4	UD1	B	5003	3	32,41,41	0.88	1 (3%)	46,62,62	1.42	3 (6%)
5	M6R	B	5004	-	15,15,15	0.69	0	14,21,21	1.17	1 (7%)
4	UD1	C	5004	3	32,41,41	0.66	0	46,62,62	1.59	3 (6%)
5	M6R	C	5005	-	15,15,15	1.10	1 (6%)	14,21,21	1.00	0
2	ACT	C	713	-	1,3,3	1.88	0	0,3,3	0.00	-
4	UD1	D	5005	3	32,41,41	0.81	1 (3%)	46,62,62	1.48	2 (4%)
5	M6R	D	5006	-	15,15,15	1.11	1 (6%)	14,21,21	0.92	1 (7%)

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
4	UD1	A	5002	3	-	0/22/63/63	0/3/3/3
5	M6R	A	5003	-	-	0/20/20/20	0/0/0/0
2	ACT	A	713	-	-	0/0/0/0	0/0/0/0
4	UD1	B	5003	3	-	0/22/63/63	0/3/3/3
5	M6R	B	5004	-	-	0/20/20/20	0/0/0/0
4	UD1	C	5004	3	-	0/22/63/63	0/3/3/3
5	M6R	C	5005	-	-	0/20/20/20	0/0/0/0
2	ACT	C	713	-	-	0/0/0/0	0/0/0/0
4	UD1	D	5005	3	-	0/22/63/63	0/3/3/3
5	M6R	D	5006	-	-	0/20/20/20	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	713	ACT	CH3-C	2.01	1.51	1.48
5	A	5003	M6R	C1-C2	2.23	1.55	1.52
4	A	5002	UD1	O4B-C1B	2.50	1.44	1.41
5	C	5005	M6R	P6-O62	2.86	1.60	1.51
5	D	5006	M6R	P6-O62	2.96	1.60	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5003	UD1	O3A-PA-O5B	-3.68	93.17	102.94
4	B	5003	UD1	PB-O3A-PA	-2.58	125.49	132.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	5005	UD1	O3A-PA-O5B	-2.53	96.22	102.94
4	A	5002	UD1	PB-O3A-PA	-2.40	125.98	132.73
4	C	5004	UD1	O6'-C6'-C5'	-2.33	103.64	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5003	M6R	1	0
5	B	5004	M6R	1	0
5	C	5005	M6R	2	0
4	D	5005	UD1	1	0
5	D	5006	M6R	1	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	338/367 (92%)	0.05	18 (5%) 30 33	12, 22, 40, 59	0
1	B	352/367 (95%)	0.03	17 (4%) 34 37	12, 22, 45, 63	0
1	C	348/367 (94%)	0.18	30 (8%) 13 14	12, 23, 51, 68	0
1	D	340/367 (92%)	0.00	16 (4%) 35 38	13, 22, 39, 47	0
All	All	1378/1468 (93%)	0.07	81 (5%) 26 29	12, 22, 45, 68	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	615	GLU	6.7
1	B	594	TYR	5.9
1	C	594	TYR	5.8
1	C	655	ALA	5.6
1	A	348	GLY	5.5

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
4	UD1	B	5003	39/39	0.95	0.14	0.55	15,23,52,55	0
2	ACT	A	713	4/4	0.87	0.16	0.48	33,34,35,35	0
5	M6R	A	5003	16/16	0.97	0.12	0.31	19,25,33,37	0
5	M6R	C	5005	16/16	0.98	0.09	0.00	19,23,36,37	0
4	UD1	D	5005	39/39	0.93	0.13	-0.02	16,24,44,47	0
4	UD1	A	5002	39/39	0.93	0.13	-0.18	19,27,44,47	0
5	M6R	B	5004	16/16	0.98	0.08	-0.41	15,20,32,34	0
3	NA	A	5001	1/1	0.96	0.10	-0.51	24,24,24,24	0
2	ACT	C	713	4/4	0.93	0.13	-0.55	40,41,41,41	0
5	M6R	D	5006	16/16	0.98	0.07	-0.60	17,24,32,34	0
4	UD1	C	5004	39/39	0.98	0.07	-0.64	13,20,26,31	0
3	NA	B	5002	1/1	0.98	0.05	-1.36	19,19,19,19	0
3	NA	D	5004	1/1	0.97	0.05	-1.80	23,23,23,23	0
3	NA	C	5003	1/1	0.98	0.04	-3.66	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.