



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:47 PM UTC

PDB ID : 1X9J / pdb_00001x9j
Title : Structure of butyrate kinase 2 reveals both open- and citrate-induced closed conformations: implications for substrate-induced fit conformational changes
Authors : Diao, J.S.; Sanders, D.A.; Hasson, M.S.
Deposited on : 2004-08-21
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

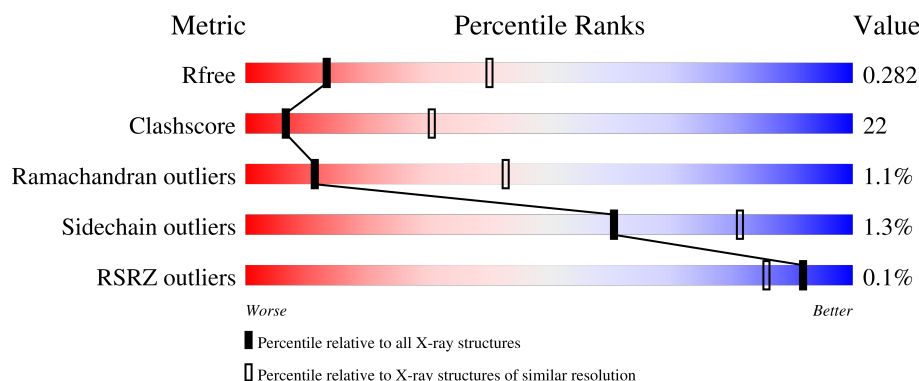
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	375	
1	B	375	
1	C	375	
1	D	375	
1	E	375	

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Mol	Chain	Length	Quality of chain
1	F	375	
1	G	375	
1	H	375	

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	GOL	A	395	-	X	-	-
2	GOL	B	394	-	X	-	-
2	GOL	C	392	-	X	-	-
2	GOL	D	393	-	X	-	-
2	GOL	F	391	-	X	-	-
5	CIT	D	381	-	X	-	-
5	CIT	D	384	-	X	-	-
5	CIT	G	382	-	X	-	-
5	CIT	G	383	-	X	-	-

2 Entry composition

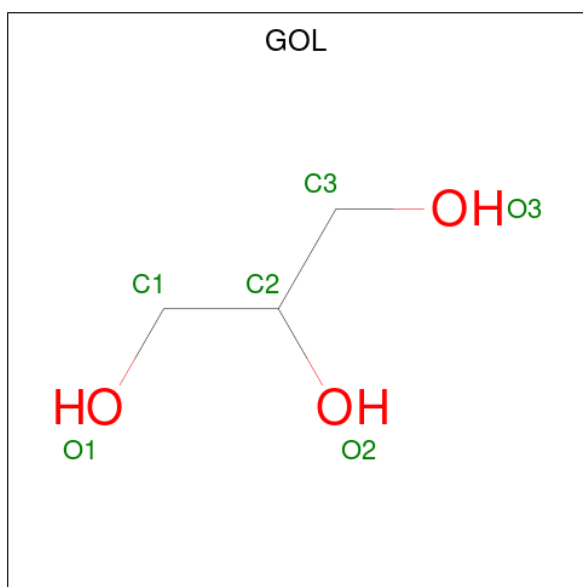
There are 6 unique types of molecules in this entry. The entry contains 23615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable butyrate kinase 2.

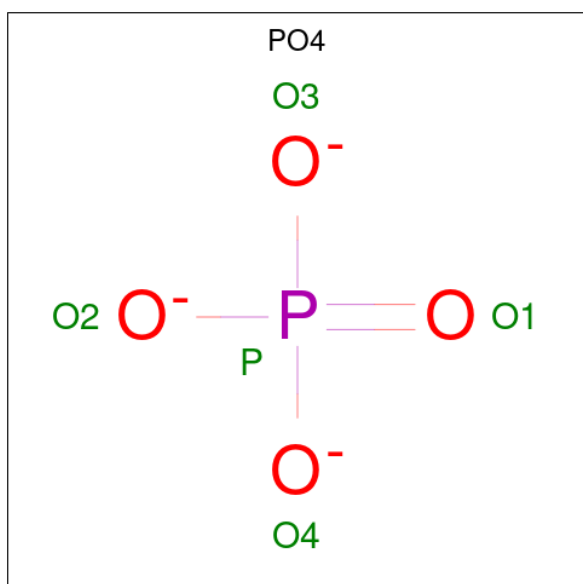
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	B	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	C	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	D	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	E	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	F	372	Total	C	N	O	S	0	0	0
			2931	1860	520	538	13			
1	G	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	H	372	Total	C	N	O	S	0	0	0
			2931	1860	520	538	13			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

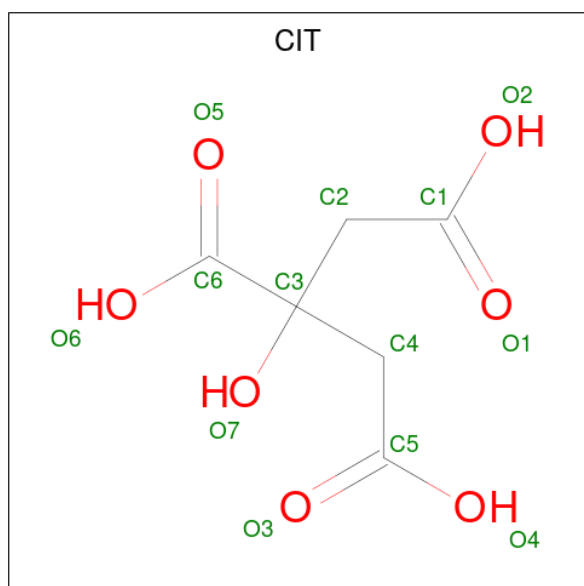


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Na 1 1	0	0

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0
5	G	1	Total C O 13 6 7	0	0
5	G	1	Total C O 13 6 7	0	0

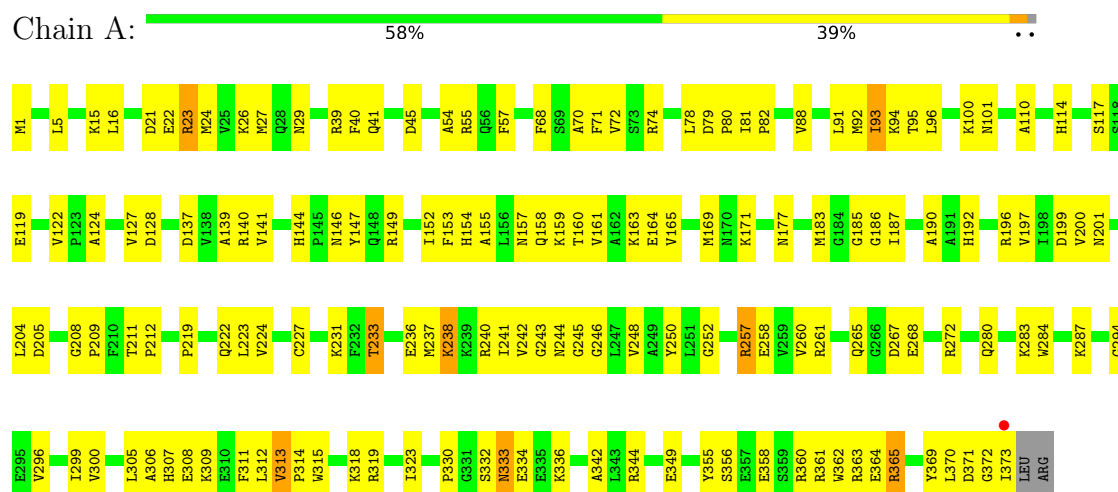
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	7	Total O 7 7	0	0
6	C	5	Total O 5 5	0	0
6	D	10	Total O 10 10	0	0
6	E	4	Total O 4 4	0	0
6	F	3	Total O 3 3	0	0
6	G	8	Total O 8 8	0	0
6	H	2	Total O 2 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Probable butyrate kinase 2





E357	W269	G185	L96	M1
E358	A270	G186	G100	L5
S359	K271	I187	N101	N8
R360	R272			
R361	V273	A190	H104	K15
W362		A191	A105	L16
R363	A278	H192		
E364	Y279		A110	D21
R365	Q280			E22
Y366		I198	H114	E23
	K283	D199		K26
L370	W284	V200	S117	M27
D371	L285			Q28
G372	G286	L204	V122	M29
I1E	L301	G208	P123	
LEU	T302	P209	A124	R39
ARG		F210	V127	F40
	L299	T211	D128	Q41
	V300	P212	P129	K42
	L301	E213		I43
	T302	R214	V132	L44
	L305		D133	D45
	A306	L223	E134	K42
	H307		M135	I43
	E308	C227	E136	L44
	K309		D137	A54
	F310	K231	V138	R55
	F311	F322	A139	Q56
	L312	T333	R140	F57
	V313			V58
	P314	E236	H144	E59
		M237	P145	E60
	K318	K238	N146	T61
		K239	Y147	
	I323	R240	Q148	S64
		I241	R149	L65
	F329	V242		S66
	P330	G243	I152	S67
		N244	F153	F68
	N333	G245	H154	S69
	E334	G246	A155	A70
	S335	L247	L156	F71
	K336	V248	N157	V72
	A337	A249	Q158	S73
	L338	Y250	K159	R74
		L251	T160	
	A342		V161	L78
	L343	A256	K162	D79
	R344	R257	K163	P80
	V345	E258	E164	I81
	L346	V259	V165	
	R347	V260	A166	V88
	G348		R167	
	E349	I263		L91
		K264	N177	M92
	P352	Q265		I93
				K94
	S356	F268	M183	T95

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	193.68Å 193.68Å 122.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.48 – 3.00 91.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (91.48-3.00) 97.2 (91.48-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.261 , 0.284 0.260 , 0.282	Depositor DCC
R_{free} test set	8832 reflections (8.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.278 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23615	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2748e-04.*

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: NA, PO4, CIT, 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	0.37	0/2997	0.85	6/4036 (0.1%)
1	B	0.36	0/2985	0.89	9/4020 (0.2%)
1	C	0.35	0/2985	0.82	1/4020 (0.0%)
1	D	0.39	0/2997	0.89	8/4036 (0.2%)
1	E	0.38	0/2985	0.86	9/4020 (0.2%)
1	F	0.41	0/2989	0.91	9/4025 (0.2%)
1	G	0.37	0/2997	0.83	1/4036 (0.0%)
1	H	0.38	0/2989	0.91	12/4025 (0.3%)
All	All	0.38	0/23924	0.87	55/32218 (0.2%)

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	GLN	OE1-CD-NE2	-10.70	111.90	122.60
1	A	41	GLN	OE1-CD-NE2	-10.19	112.41	122.60
1	H	46	GLN	OE1-CD-NE2	-10.00	112.60	122.60
1	F	41	GLN	OE1-CD-NE2	-9.99	112.61	122.60
1	B	46	GLN	OE1-CD-NE2	-9.96	112.64	122.60

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	2939	0	2969	122	0
1	B	2927	0	2955	139	0
1	C	2927	0	2955	139	0
1	D	2939	0	2969	141	0
1	E	2927	0	2955	147	0
1	F	2931	0	2958	132	0
1	G	2939	0	2969	135	0
1	H	2931	0	2958	142	0
2	A	6	0	4	0	0
2	B	6	0	4	0	0
2	C	6	0	4	0	0
2	D	6	0	4	0	0
2	F	6	0	4	0	0
3	B	5	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	D	1	0	0	0	0
5	D	26	0	10	3	0
5	G	26	0	10	0	0
6	A	8	0	0	1	0
6	B	7	0	0	1	0
6	C	5	0	0	0	0
6	D	10	0	0	0	0
6	E	4	0	0	0	0
6	F	3	0	0	0	0
6	G	8	0	0	0	0
6	H	2	0	0	0	0
All	All	23615	0	23728	1020	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 22.

The worst 5 of 1020 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:24:MET:HE1	1:B:24:MET:HE1	1.42	1.01
1:A:88:VAL:HG12	1:A:93:ILE:HD11	1.43	1.00
1:A:27:MET:HG2	1:B:24:MET:HE3	1.52	0.92
1:A:257:ARG:HB3	1:A:257:ARG:HH11	1.35	0.91
1:D:88:VAL:HG12	1:D:93:ILE:HD11	1.53	0.90

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	371/375 (99%)	325 (88%)	39 (10%)	7 (2%)	6	30
1	B	369/375 (98%)	326 (88%)	39 (11%)	4 (1%)	11	43
1	C	369/375 (98%)	325 (88%)	38 (10%)	6 (2%)	7	34
1	D	371/375 (99%)	327 (88%)	41 (11%)	3 (1%)	16	50
1	E	369/375 (98%)	325 (88%)	40 (11%)	4 (1%)	11	43
1	F	370/375 (99%)	325 (88%)	43 (12%)	2 (0%)	24	60
1	G	371/375 (99%)	322 (87%)	45 (12%)	4 (1%)	11	43
1	H	370/375 (99%)	326 (88%)	41 (11%)	3 (1%)	16	50
All	All	2960/3000 (99%)	2601 (88%)	326 (11%)	33 (1%)	11	43

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	LEU
1	H	60	GLU
1	A	39	ARG
1	A	243	GLY
1	C	245	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	313/315 (99%)	308 (98%)	5 (2%)	55	79
1	B	312/315 (99%)	309 (99%)	3 (1%)	68	84
1	C	312/315 (99%)	309 (99%)	3 (1%)	68	84
1	D	313/315 (99%)	309 (99%)	4 (1%)	61	81
1	E	312/315 (99%)	308 (99%)	4 (1%)	61	81
1	F	312/315 (99%)	306 (98%)	6 (2%)	50	76
1	G	313/315 (99%)	310 (99%)	3 (1%)	68	84
1	H	312/315 (99%)	308 (99%)	4 (1%)	61	81
All	All	2499/2520 (99%)	2467 (99%)	32 (1%)	61	81

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	23	ARG
1	H	135	MET
1	D	136	GLU
1	D	48	GLU
1	H	238	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	307	HIS
1	H	148	GLN
1	E	265	GLN
1	H	146	ASN
1	G	333	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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
3	PO4	F	403	-	4,4,4	1.46	1 (25%)	6,6,6	0.89	0
2	GOL	A	395	-	5,5,5	4.65	5 (100%)	5,5,5	5.80	4 (80%)
5	CIT	G	383	-	12,12,12	1.89	5 (41%)	17,17,17	3.05	8 (47%)
5	CIT	G	382	-	12,12,12	1.80	4 (33%)	17,17,17	3.12	9 (52%)
2	GOL	F	391	-	5,5,5	4.62	5 (100%)	5,5,5	5.70	4 (80%)
2	GOL	C	392	-	5,5,5	4.65	5 (100%)	5,5,5	5.79	4 (80%)
3	PO4	H	404	-	4,4,4	1.51	1 (25%)	6,6,6	0.89	0
5	CIT	D	384	-	12,12,12	1.85	4 (33%)	17,17,17	3.00	8 (47%)
3	PO4	B	402	-	4,4,4	1.44	1 (25%)	6,6,6	0.90	0
3	PO4	E	401	-	4,4,4	1.42	1 (25%)	6,6,6	0.93	0
2	GOL	B	394	-	5,5,5	4.68	5 (100%)	5,5,5	5.79	4 (80%)
3	PO4	E	405	-	4,4,4	1.46	1 (25%)	6,6,6	0.90	0
5	CIT	D	381	-	12,12,12	1.83	4 (33%)	17,17,17	2.75	8 (47%)
2	GOL	D	393	-	5,5,5	4.75	5 (100%)	5,5,5	5.97	4 (80%)

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	395	-	-	4/4/4/4	-
5	CIT	G	383	-	-	7/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	G	382	-	-	10/16/16/16	-
2	GOL	F	391	-	-	2/4/4/4	-
2	GOL	C	392	-	-	3/4/4/4	-
5	CIT	D	384	-	-	7/16/16/16	-
2	GOL	B	394	-	-	2/4/4/4	-
5	CIT	D	381	-	-	6/16/16/16	-
2	GOL	D	393	-	-	3/4/4/4	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	393	GOL	C3-C2	-7.71	1.22	1.51
2	A	395	GOL	C3-C2	-7.51	1.23	1.51
2	C	392	GOL	C3-C2	-7.46	1.23	1.51
2	B	394	GOL	C3-C2	-7.46	1.23	1.51
2	F	391	GOL	C3-C2	-7.43	1.23	1.51

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	393	GOL	O3-C3-C2	11.36	161.50	110.38
2	C	392	GOL	O3-C3-C2	11.24	160.98	110.38
2	B	394	GOL	O3-C3-C2	11.19	160.73	110.38
2	A	395	GOL	O3-C3-C2	11.13	160.50	110.38
2	F	391	GOL	O3-C3-C2	11.04	160.08	110.38

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	395	GOL	O1-C1-C2-C3
2	A	395	GOL	C1-C2-C3-O3
2	B	394	GOL	C1-C2-C3-O3
2	C	392	GOL	C1-C2-C3-O3
2	D	393	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	381	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(Å ²)	Q<0.9
1	A	373/375 (99%)	-1.41	1 (0%) 90 79	14, 49, 111, 139	0
1	B	371/375 (98%)	-1.31	0 100 100	10, 52, 117, 136	0
1	C	371/375 (98%)	-1.38	0 100 100	15, 47, 105, 138	0
1	D	373/375 (99%)	-1.42	1 (0%) 90 79	18, 39, 109, 140	0
1	E	371/375 (98%)	-1.45	0 100 100	20, 43, 101, 135	0
1	F	372/375 (99%)	-1.36	0 100 100	23, 49, 105, 143	0
1	G	373/375 (99%)	-1.40	0 100 100	23, 46, 113, 142	0
1	H	372/375 (99%)	-1.34	0 100 100	21, 54, 117, 146	0
All	All	2976/3000 (99%)	-1.38	2 (0%) 92 86	10, 48, 111, 146	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	ILE	2.3
1	D	373	ILE	2.2

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

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(Å ²)	Q<0.9
2	GOL	B	394	6/6	0.94	0.11	54,54,55,55	0
2	GOL	A	395	6/6	0.98	0.08	68,71,71,71	0
5	CIT	G	383	13/13	0.98	0.06	88,92,95,96	0
2	GOL	D	393	6/6	0.99	0.04	43,44,46,49	0
2	GOL	F	391	6/6	0.99	0.04	56,58,59,59	0
3	PO4	B	402	5/5	0.99	0.05	83,83,83,84	0
3	PO4	E	401	5/5	0.99	0.06	76,76,77,78	0
3	PO4	E	405	5/5	0.99	0.07	97,98,98,99	0
3	PO4	F	403	5/5	0.99	0.06	98,99,99,100	0
3	PO4	H	404	5/5	0.99	0.04	76,77,78,78	0
4	NA	D	380	1/1	0.99	0.03	24,24,24,24	0
5	CIT	D	381	13/13	0.99	0.06	78,80,81,81	0
5	CIT	D	384	13/13	0.99	0.07	89,91,92,92	0
5	CIT	G	382	13/13	0.99	0.06	67,68,69,70	0
2	GOL	C	392	6/6	0.99	0.07	40,43,44,44	0

6.5 Other polymers

There are no such residues in this entry.