



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:34 PM UTC

PDB ID : 8SYJ / pdb_00008syj
Title : Structure of apurinic/apyrimidinic DNA lyase TK0353 from *Thermococcus kodakarensis* (Iodide crystal form)
Authors : Eckenroth, B.E.; Gardner, A.F.; Doubie, S.
Deposited on : 2023-05-25
Resolution : 2.20 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

<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

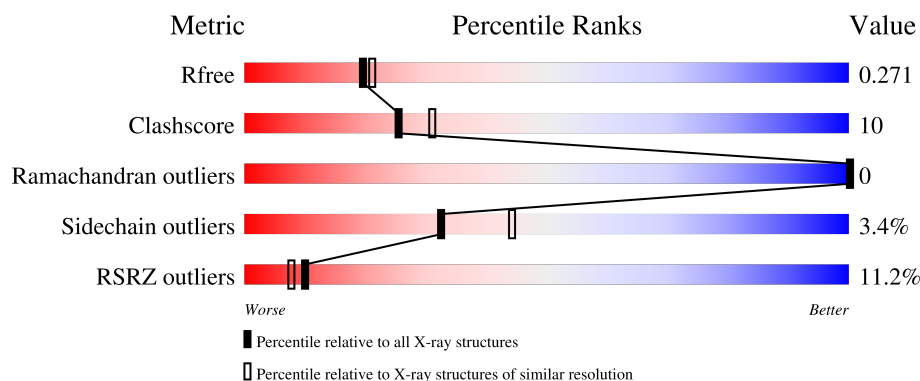
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	170	3% 79% 20% ..
1	B	170	14% 78% 18% ..
1	C	170	16% 82% 15% ..
1	D	170	12% 80% 18% ..

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	IOD	C	211	-	-	X	-
2	IOD	D	201	-	-	X	-
3	GOL	B	213	-	-	X	-
4	SO4	A	221	-	-	X	-
4	SO4	D	212	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5513 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 TK0353.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	5	0
			1360	871	237	240	12			
1	B	165	Total	C	N	O	S	0	2	0
			1270	819	214	227	10			
1	C	165	Total	C	N	O	S	0	2	0
			1256	812	209	224	11			
1	D	169	Total	C	N	O	S	0	4	0
			1321	849	226	233	13			

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

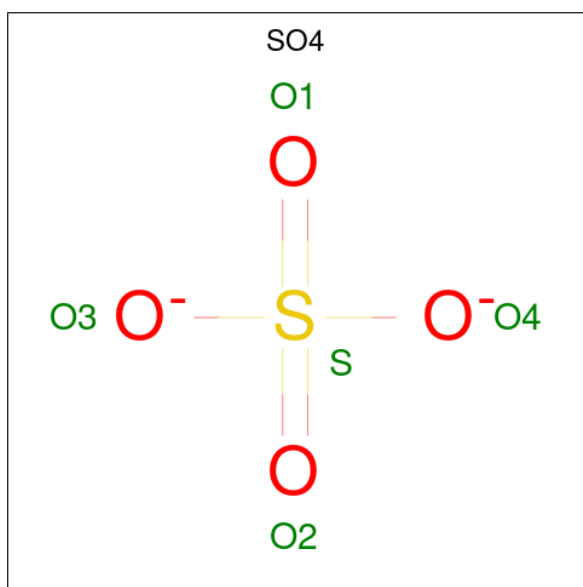
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	I	0	3
			15	15		
2	B	12	Total	I	0	2
			14	14		
2	C	12	Total	I	0	0
			12	12		
2	D	10	Total	I	0	0
			10	10		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	38	Total	O	0	0
			38	38		
5	C	27	Total	O	0	0
			27	27		

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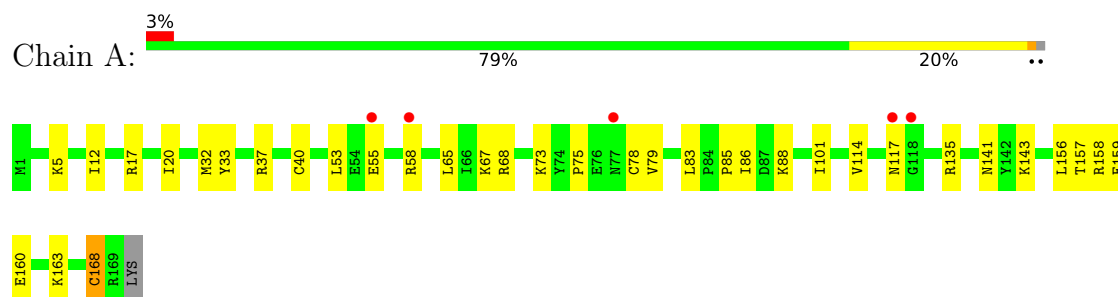
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	47	Total	O	0	0
			47	47		

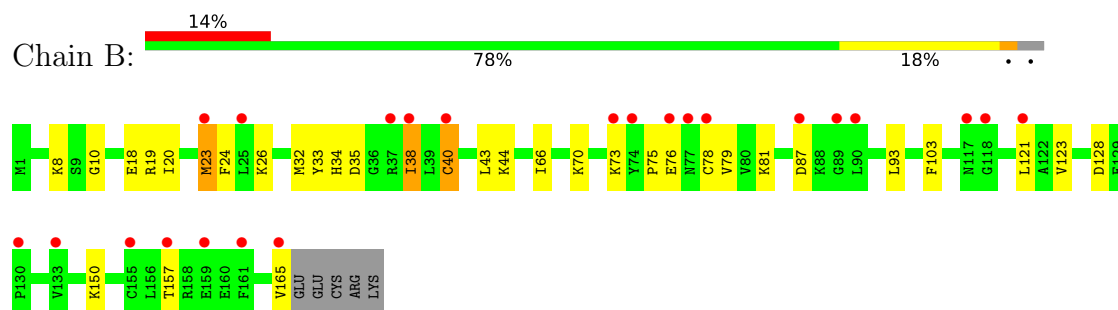
3 Residue-property plots [i](#)

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.

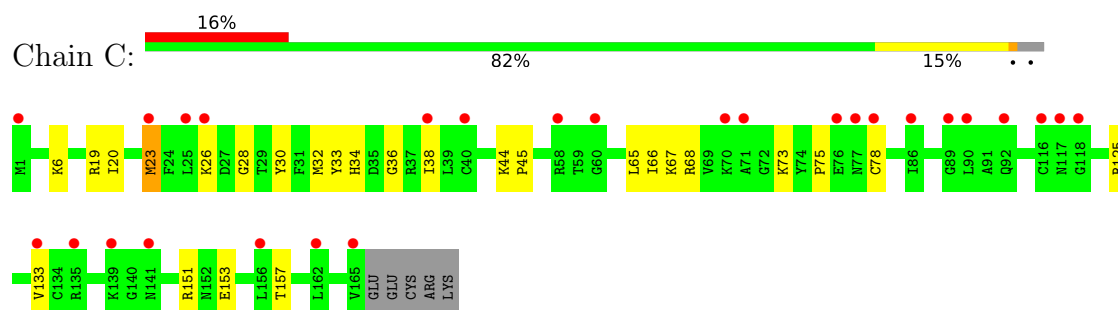
• Molecule 1: TK0353



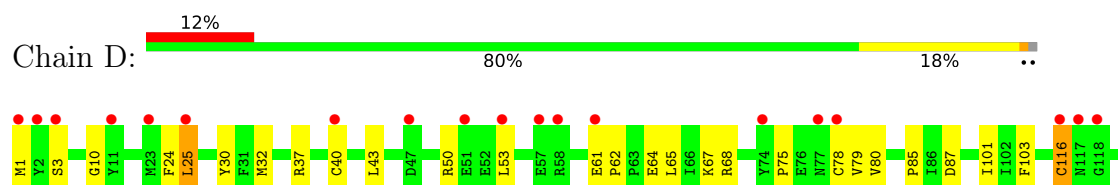
• Molecule 1: TK0353

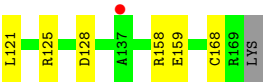


• Molecule 1: TK0353



• Molecule 1: TK0353





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.55Å 89.12Å 128.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.49 – 2.20 38.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.49-2.20) 99.8 (38.49-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.260 0.238 , 0.271	Depositor DCC
R_{free} test set	3754 reflections (8.69%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtrriage
Anisotropy	0.571	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5513	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.42 % 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 2.3686e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, GOL, IOD

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	0.28	0/1402	0.51	0/1887
1	B	0.26	0/1303	0.51	0/1764
1	C	0.24	0/1289	0.51	0/1747
1	D	0.27	0/1360	0.51	0/1837
All	All	0.26	0/5354	0.51	0/7235

There are no bond length outliers.

There are no bond angle outliers.

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	1360	0	1377	28	0
1	B	1270	0	1250	28	0
1	C	1256	0	1227	23	0
1	D	1321	0	1307	25	0
2	A	15	0	0	4	0
2	B	14	0	0	2	0
2	C	12	0	0	5	0
2	D	10	0	0	2	0
3	A	36	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	5	0
3	C	6	0	8	2	0
3	D	6	0	8	0	0
4	A	15	0	0	3	0
4	B	10	0	0	1	0
4	C	5	0	0	0	0
4	D	15	0	0	3	0
5	A	38	0	0	2	0
5	B	38	0	0	2	0
5	C	27	0	0	2	0
5	D	47	0	0	2	0
All	All	5513	0	5241	102	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 10.

All (102) 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:117:ASN:ND2	1:A:168[B]:CYS:SG	2.39	0.94
1:A:85:PRO:HG3	1:D:85:PRO:HG3	1.54	0.90
1:D:158:ARG:NH2	4:D:212:SO4:O2	2.11	0.82
1:B:44:LYS:NZ	3:B:213:GOL:O3	2.15	0.74
1:A:158:ARG:NH2	4:A:221:SO4:S	2.61	0.74
4:D:214:SO4:O3	5:D:301:HOH:O	2.06	0.73
1:C:151:ARG:NH1	1:C:153:GLU:OE2	2.25	0.70
1:B:73:LYS:HE3	5:B:318:HOH:O	1.96	0.65
1:A:32:MET:HE3	2:A:201[B]:IOD:I	2.67	0.64
1:A:88:LYS:NZ	5:A:301:HOH:O	2.12	0.63
3:B:213:GOL:O3	3:B:213:GOL:O1	2.09	0.63
1:A:160:GLU:HA	1:A:163:LYS:HE3	1.79	0.62
1:D:67:LYS:HG2	2:D:201:IOD:I	2.71	0.61
1:A:158:ARG:NH2	4:A:221:SO4:O4	2.34	0.61
1:A:65:LEU:HD11	1:A:75:PRO:HG3	1.81	0.60
1:D:62:PRO:HG2	2:D:201:IOD:I	2.72	0.59
1:A:67:LYS:HG2	2:A:205:IOD:I	2.73	0.58
1:A:37:ARG:NH1	1:A:83:LEU:O	2.37	0.58
1:A:55:GLU:OE1	5:A:302:HOH:O	2.17	0.58
1:B:19:ARG:HG2	1:B:32:MET:HE1	1.85	0.57
1:D:25:LEU:HD22	1:D:30:TYR:CD1	2.40	0.57
1:C:68:ARG:HB3	1:C:73:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HG12	1:A:33:TYR:HD1	1.70	0.56
1:A:32:MET:HG3	1:A:101:ILE:HD13	1.87	0.55
1:A:141:ASN:OD1	1:A:143:LYS:HE3	2.07	0.54
1:B:26:LYS:NZ	3:B:213:GOL:H12	2.22	0.54
3:C:213:GOL:O3	5:C:301:HOH:O	2.05	0.54
1:C:75:PRO:HG2	1:C:78[B]:CYS:SG	2.46	0.54
1:A:159:GLU:H	1:A:159:GLU:CD	2.16	0.54
1:C:26:LYS:C	1:C:28:GLY:H	2.15	0.54
1:A:75:PRO:HG2	1:A:78[B]:CYS:SG	2.48	0.54
1:B:103:PHE:HA	1:D:43:LEU:HD12	1.88	0.54
1:B:23:MET:N	1:B:23:MET:HE2	2.24	0.53
2:B:201:IOD:I	1:D:25:LEU:HB3	2.80	0.52
1:D:10:GLY:HA2	1:D:24:PHE:CE2	2.45	0.52
1:B:8:LYS:N	3:B:214:GOL:H2	2.25	0.52
1:D:40[A]:CYS:HA	1:D:79:VAL:O	2.10	0.52
1:A:86:ILE:HB	1:D:37:ARG:HG2	1.92	0.52
1:B:26:LYS:HZ3	3:B:213:GOL:H12	1.74	0.51
1:A:65:LEU:HA	3:A:216:GOL:H11	1.92	0.51
1:C:151:ARG:HD2	2:C:212:IOD:I	2.80	0.51
1:B:40[A]:CYS:HA	1:B:79:VAL:O	2.12	0.50
1:D:87:ASP:OD1	1:D:125[B]:ARG:NH2	2.30	0.50
1:A:156:LEU:HG	2:A:212[A]:IOD:I	2.81	0.50
1:C:26:LYS:O	2:C:209:IOD:I	3.00	0.50
1:D:40[B]:CYS:HA	1:D:79:VAL:O	2.11	0.50
1:C:23:MET:HB3	5:C:315:HOH:O	2.10	0.50
1:C:125:ARG:HG2	1:C:133:VAL:HG22	1.94	0.50
1:B:20:ILE:HD13	1:B:66:ILE:HG21	1.94	0.49
1:B:93:LEU:HD11	1:B:165:VAL:HG13	1.94	0.49
1:B:40[B]:CYS:HA	1:B:79:VAL:O	2.12	0.49
1:D:50:ARG:HA	1:D:53:LEU:HB2	1.94	0.49
1:A:17:ARG:HD3	1:A:86:ILE:HD11	1.95	0.49
1:D:65:LEU:HD11	1:D:75:PRO:HG3	1.94	0.49
1:C:20:ILE:HG12	1:C:33:TYR:HD1	1.78	0.48
1:B:73:LYS:NZ	4:B:215:SO4:O4	2.28	0.48
1:B:128:ASP:OD2	1:D:128:ASP:HB3	2.14	0.48
1:D:40[A]:CYS:HB3	1:D:78:CYS:SG	2.54	0.47
1:D:116:CYS:SG	1:D:168[B]:CYS:HB3	2.54	0.47
1:A:159:GLU:HG3	2:A:207:IOD:I	2.84	0.47
1:C:68:ARG:HD2	2:C:211:IOD:I	2.84	0.47
1:C:20:ILE:HD13	1:C:66:ILE:HG21	1.95	0.47
1:D:159:GLU:H	1:D:159:GLU:CD	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PRO:HG2	1:B:78[B]:CYS:SG	2.55	0.46
1:B:79:VAL:HA	5:B:317:HOH:O	2.15	0.46
1:C:36:GLY:HA3	3:C:213:GOL:H32	1.97	0.46
1:B:38:ILE:HD13	1:B:38:ILE:HA	1.80	0.46
1:D:64:GLU:O	1:D:68:ARG:HG3	2.16	0.46
1:C:19:ARG:HG2	1:C:32:MET:HE1	1.98	0.46
1:A:135:ARG:NH2	4:A:221:SO4:O3	2.46	0.45
1:C:44:LYS:HA	1:C:44:LYS:HD3	1.70	0.45
1:D:32:MET:HG3	1:D:101:ILE:HD13	1.99	0.45
1:A:5:LYS:HD3	1:A:12:ILE:HD12	1.98	0.45
1:B:26:LYS:NZ	1:D:103:PHE:O	2.50	0.45
1:A:68:ARG:NH1	1:A:73:LYS:HD3	2.32	0.45
1:A:157:THR:OG1	1:A:160:GLU:HG3	2.16	0.45
1:C:65:LEU:HA	2:C:211:IOD:I	2.87	0.44
1:B:70:LYS:HD3	2:B:209[A]:IOD:I	2.87	0.44
1:B:87:ASP:OD2	1:B:123:VAL:HG21	2.18	0.44
1:B:23:MET:HE3	1:B:103:PHE:CD2	2.53	0.44
1:C:32:MET:HG2	1:C:33:TYR:N	2.33	0.44
1:B:150:LYS:HD2	5:D:307:HOH:O	2.17	0.43
1:C:23:MET:HE3	1:C:23:MET:HB2	1.84	0.43
1:B:23:MET:HE2	1:B:23:MET:H	1.82	0.43
1:A:40[B]:CYS:HA	1:A:79:VAL:O	2.19	0.43
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.83	0.43
1:B:10:GLY:HA2	1:B:24:PHE:CE2	2.54	0.43
1:B:32:MET:HG2	1:B:33:TYR:N	2.33	0.43
1:D:121:LEU:HD11	1:D:168[B]:CYS:SG	2.59	0.43
1:B:81:LYS:NZ	1:B:128:ASP:OD2	2.52	0.42
1:B:18:GLU:OE2	1:B:70:LYS:NZ	2.50	0.42
1:C:26:LYS:C	1:C:28:GLY:N	2.78	0.42
1:D:40[B]:CYS:SG	1:D:80:VAL:HG22	2.60	0.42
1:D:125[A]:ARG:NH2	4:D:212:SO4:O3	2.51	0.42
1:C:67:LYS:HG2	2:C:208:IOD:I	2.90	0.41
1:A:40[A]:CYS:HA	1:A:79:VAL:O	2.20	0.41
1:C:68:ARG:HA	1:C:73:LYS:HD2	2.03	0.41
1:C:19:ARG:HB3	1:C:34:HIS:CD2	2.56	0.41
1:D:61:GLU:HA	1:D:62:PRO:HD3	1.94	0.41
1:C:30:TYR:CZ	1:C:45:PRO:HD3	2.56	0.40
1:C:44:LYS:HD2	1:C:45:PRO:HD2	2.03	0.40
1:B:34:HIS:HD2	1:B:35:ASP:O	2.04	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	172/170 (101%)	169 (98%)	3 (2%)	0	100	100
1	B	165/170 (97%)	162 (98%)	3 (2%)	0	100	100
1	C	165/170 (97%)	159 (96%)	6 (4%)	0	100	100
1	D	170/170 (100%)	168 (99%)	2 (1%)	0	100	100
All	All	672/680 (99%)	658 (98%)	14 (2%)	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	147/151 (97%)	142 (97%)	5 (3%)	32	44
1	B	132/151 (87%)	124 (94%)	8 (6%)	17	20
1	C	129/151 (85%)	125 (97%)	4 (3%)	35	48
1	D	138/151 (91%)	133 (96%)	5 (4%)	31	42
All	All	546/604 (90%)	524 (96%)	22 (4%)	32	38

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58[A]	ARG
1	A	58[B]	ARG

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Mol	Chain	Res	Type
1	A	114	VAL
1	A	168[A]	CYS
1	A	168[B]	CYS
1	B	23	MET
1	B	38	ILE
1	B	40[A]	CYS
1	B	40[B]	CYS
1	B	43	LEU
1	B	76	GLU
1	B	121	LEU
1	B	157	THR
1	C	6	LYS
1	C	23	MET
1	C	38	ILE
1	C	157	THR
1	D	1[A]	MET
1	D	1[B]	MET
1	D	3	SER
1	D	25	LEU
1	D	116	CYS

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

Mol	Chain	Res	Type
1	A	77	ASN
1	B	34	HIS
1	B	152	ASN
1	D	77	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 70 ligands modelled in this entry, 51 are monoatomic - leaving 19 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	SO4	D	213	-	4,4,4	0.22	0	6,6,6	0.47	0
3	GOL	C	213	-	5,5,5	0.82	0	5,5,5	1.23	1 (20%)
3	GOL	A	216	-	5,5,5	1.17	1 (20%)	5,5,5	0.88	0
4	SO4	A	220	-	4,4,4	0.25	0	6,6,6	0.32	0
4	SO4	B	216	-	4,4,4	0.20	0	6,6,6	0.46	0
3	GOL	D	211	-	5,5,5	1.15	0	5,5,5	0.95	0
4	SO4	D	212	-	4,4,4	0.24	0	6,6,6	0.23	0
4	SO4	A	221	-	4,4,4	0.25	0	6,6,6	0.16	0
3	GOL	A	214	-	5,5,5	1.30	1 (20%)	5,5,5	0.87	0
3	GOL	A	217	-	5,5,5	1.23	1 (20%)	5,5,5	1.07	0
3	GOL	A	213	-	5,5,5	1.22	0	5,5,5	1.07	0
4	SO4	A	219	-	4,4,4	0.24	0	6,6,6	0.15	0
4	SO4	B	215	-	4,4,4	0.28	0	6,6,6	0.23	0
3	GOL	A	215	-	5,5,5	0.98	0	5,5,5	0.99	0
4	SO4	D	214	-	4,4,4	0.19	0	6,6,6	0.39	0
4	SO4	C	214	-	4,4,4	0.23	0	6,6,6	0.45	0
3	GOL	A	218	-	5,5,5	0.81	0	5,5,5	1.18	0
3	GOL	B	214	-	5,5,5	0.93	0	5,5,5	1.09	0
3	GOL	B	213	-	5,5,5	1.13	0	5,5,5	1.24	1 (20%)

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	GOL	A	214	-	-	4/4/4/4	-
3	GOL	C	213	-	-	4/4/4/4	-
3	GOL	A	217	-	-	2/4/4/4	-
3	GOL	A	216	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	213	-	-	0/4/4/4	-
3	GOL	A	218	-	-	2/4/4/4	-
3	GOL	D	211	-	-	2/4/4/4	-
3	GOL	A	215	-	-	0/4/4/4	-
3	GOL	B	214	-	-	3/4/4/4	-
3	GOL	B	213	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	217	GOL	O2-C2	-2.17	1.37	1.43
3	A	214	GOL	O2-C2	-2.09	1.37	1.43
3	A	216	GOL	O2-C2	-2.01	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	213	GOL	C3-C2-C1	-2.14	103.94	111.80
3	C	213	GOL	C3-C2-C1	-2.05	104.29	111.80

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	217	GOL	C1-C2-C3-O3
3	A	218	GOL	O1-C1-C2-C3
3	B	214	GOL	O1-C1-C2-C3
3	C	213	GOL	C1-C2-C3-O3
3	A	218	GOL	O1-C1-C2-O2
3	B	214	GOL	O1-C1-C2-O2
3	A	214	GOL	O1-C1-C2-C3
3	A	214	GOL	C1-C2-C3-O3
3	C	213	GOL	O1-C1-C2-C3
3	D	211	GOL	C1-C2-C3-O3
3	A	217	GOL	O2-C2-C3-O3
3	C	213	GOL	O2-C2-C3-O3
3	A	214	GOL	O2-C2-C3-O3
3	A	214	GOL	O1-C1-C2-O2
3	B	214	GOL	O2-C2-C3-O3
3	D	211	GOL	O2-C2-C3-O3
3	C	213	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	213	GOL	2	0
3	A	216	GOL	1	0
4	D	212	SO4	2	0
4	A	221	SO4	3	0
4	B	215	SO4	1	0
4	D	214	SO4	1	0
3	B	214	GOL	1	0
3	B	213	GOL	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	169/170 (99%)	0.62	5 (2%) 52 49	25, 47, 67, 94	6 (3%)
1	B	165/170 (97%)	0.98	23 (13%) 6 5	31, 53, 93, 123	2 (1%)
1	C	165/170 (97%)	1.17	27 (16%) 4 3	34, 58, 93, 110	2 (1%)
1	D	169/170 (99%)	0.89	20 (11%) 9 7	22, 52, 81, 105	4 (2%)
All	All	668/680 (98%)	0.91	75 (11%) 10 8	22, 53, 86, 123	14 (2%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	GLY	5.0
1	C	76	GLU	4.5
1	D	1[A]	MET	4.5
1	B	159	GLU	4.0
1	B	157	THR	3.9
1	C	1	MET	3.8
1	B	117	ASN	3.8
1	C	40[A]	CYS	3.4
1	B	165	VAL	3.4
1	C	89	GLY	3.3
1	B	40[A]	CYS	3.3
1	C	133	VAL	3.2
1	C	162	LEU	3.2
1	C	90	LEU	3.1
1	B	161	PHE	3.1
1	C	78[A]	CYS	3.0
1	C	139	LYS	3.0
1	B	87	ASP	2.9
1	B	38	ILE	2.9
1	D	61	GLU	2.9
1	D	23	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	73	LYS	2.8
1	C	25	LEU	2.8
1	A	77	ASN	2.8
1	C	117	ASN	2.8
1	C	77	ASN	2.7
1	B	37	ARG	2.7
1	B	76	GLU	2.7
1	D	137	ALA	2.6
1	D	117	ASN	2.6
1	C	86	ILE	2.6
1	D	58	ARG	2.5
1	B	77	ASN	2.5
1	C	60	GLY	2.5
1	C	118	GLY	2.5
1	C	165	VAL	2.5
1	B	74	TYR	2.5
1	D	47	ASP	2.5
1	C	135	ARG	2.4
1	B	133	VAL	2.4
1	D	51	GLU	2.4
1	B	78[A]	CYS	2.4
1	C	70	LYS	2.4
1	D	74	TYR	2.3
1	B	90	LEU	2.3
1	C	38	ILE	2.3
1	D	78	CYS	2.3
1	A	118	GLY	2.3
1	B	118	GLY	2.2
1	A	55	GLU	2.2
1	C	26	LYS	2.2
1	B	25	LEU	2.2
1	D	116	CYS	2.2
1	D	53	LEU	2.2
1	C	141	ASN	2.2
1	D	77	ASN	2.2
1	B	155	CYS	2.2
1	D	40[A]	CYS	2.2
1	D	2	TYR	2.1
1	C	156	LEU	2.1
1	B	23	MET	2.1
1	C	23	MET	2.1
1	B	130	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	58[A]	ARG	2.1
1	D	118	GLY	2.1
1	D	25	LEU	2.1
1	C	116	CYS	2.1
1	B	121	LEU	2.1
1	C	71	ALA	2.0
1	D	57	GLU	2.0
1	C	92	GLN	2.0
1	A	117	ASN	2.0
1	D	11	TYR	2.0
1	D	3	SER	2.0
1	C	58	ARG	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(Å ²)	Q<0.9
4	SO4	A	221	5/5	0.73	0.13	84,85,91,98	0
3	GOL	D	211	6/6	0.75	0.18	50,53,67,68	0
3	GOL	A	215	6/6	0.76	0.18	39,55,59,69	0
4	SO4	D	212	5/5	0.76	0.13	75,81,88,91	0
3	GOL	A	218	6/6	0.78	0.14	52,57,61,63	0
4	SO4	D	213	5/5	0.79	0.21	54,56,65,74	0
3	GOL	A	214	6/6	0.80	0.18	46,55,65,69	0
3	GOL	C	213	6/6	0.81	0.14	54,59,66,70	0
3	GOL	A	213	6/6	0.83	0.13	51,54,58,63	0
3	GOL	A	217	6/6	0.84	0.18	49,55,64,68	0
3	GOL	A	216	6/6	0.86	0.14	51,56,60,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	B	211	1/1	0.86	0.26	73,73,73,73	1
2	IOD	D	201	1/1	0.87	0.16	102,102,102,102	0
2	IOD	C	211	1/1	0.87	0.20	95,95,95,95	0
4	SO4	C	214	5/5	0.88	0.16	34,52,60,62	0
2	IOD	D	205	1/1	0.89	0.15	81,81,81,81	0
3	GOL	B	214	6/6	0.89	0.15	34,58,60,65	0
4	SO4	A	220	5/5	0.90	0.11	57,62,69,81	0
4	SO4	B	215	5/5	0.91	0.10	58,64,75,76	0
3	GOL	B	213	6/6	0.91	0.10	40,50,51,56	0
2	IOD	A	208[A]	1/1	0.91	0.12	67,67,67,67	1
2	IOD	A	208[B]	1/1	0.91	0.12	57,57,57,57	1
2	IOD	A	212[B]	1/1	0.92	0.11	60,60,60,60	1
2	IOD	D	207	1/1	0.92	0.10	66,66,66,66	0
2	IOD	B	210	1/1	0.92	0.09	57,57,57,57	1
2	IOD	A	204	1/1	0.92	0.08	68,68,68,68	1
2	IOD	A	210	1/1	0.92	0.12	61,61,61,61	1
2	IOD	A	212[A]	1/1	0.92	0.11	46,46,46,46	1
2	IOD	B	209[B]	1/1	0.93	0.08	71,71,71,71	1
4	SO4	B	216	5/5	0.93	0.13	30,34,62,65	0
4	SO4	A	219	5/5	0.93	0.19	53,65,67,76	0
2	IOD	C	201	1/1	0.93	0.18	71,71,71,71	0
2	IOD	B	209[A]	1/1	0.93	0.08	66,66,66,66	1
2	IOD	C	212	1/1	0.94	0.12	72,72,72,72	0
2	IOD	A	207	1/1	0.94	0.10	87,87,87,87	0
2	IOD	C	210	1/1	0.95	0.12	59,59,59,59	0
2	IOD	D	203	1/1	0.95	0.12	65,65,65,65	0
2	IOD	B	202	1/1	0.95	0.15	92,92,92,92	0
2	IOD	A	209	1/1	0.95	0.18	81,81,81,81	0
2	IOD	D	208	1/1	0.95	0.21	84,84,84,84	0
2	IOD	D	210	1/1	0.95	0.20	90,90,90,90	0
4	SO4	D	214	5/5	0.95	0.12	37,51,61,74	0
2	IOD	D	209	1/1	0.96	0.19	61,61,61,61	0
2	IOD	C	203	1/1	0.96	0.12	84,84,84,84	0
2	IOD	C	206	1/1	0.96	0.10	63,63,63,63	0
2	IOD	D	204	1/1	0.96	0.12	83,83,83,83	0
2	IOD	A	211	1/1	0.96	0.07	52,52,52,52	1
2	IOD	B	212	1/1	0.96	0.09	50,50,50,50	1
2	IOD	B	201	1/1	0.96	0.09	70,70,70,70	0
2	IOD	C	202	1/1	0.97	0.10	61,61,61,61	0
2	IOD	B	204[B]	1/1	0.97	0.12	62,62,62,62	1
2	IOD	C	204	1/1	0.97	0.21	81,81,81,81	0
2	IOD	B	206	1/1	0.97	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	C	208	1/1	0.97	0.20	85,85,85,85	0
2	IOD	A	205	1/1	0.97	0.11	98,98,98,98	0
2	IOD	B	204[A]	1/1	0.97	0.12	49,49,49,49	1
2	IOD	B	205	1/1	0.98	0.09	58,58,58,58	0
2	IOD	C	207	1/1	0.98	0.18	79,79,79,79	0
2	IOD	A	202	1/1	0.98	0.11	52,52,52,52	0
2	IOD	D	206	1/1	0.98	0.23	82,82,82,82	0
2	IOD	B	207	1/1	0.98	0.10	63,63,63,63	0
2	IOD	B	203	1/1	0.98	0.09	53,53,53,53	0
2	IOD	A	203	1/1	0.98	0.09	60,60,60,60	0
2	IOD	A	206	1/1	0.98	0.13	65,65,65,65	0
2	IOD	D	202	1/1	0.98	0.09	70,70,70,70	0
2	IOD	A	201[A]	1/1	0.99	0.07	41,41,41,41	1
2	IOD	B	208	1/1	0.99	0.09	63,63,63,63	0
2	IOD	C	209	1/1	0.99	0.13	52,52,52,52	0
2	IOD	C	205	1/1	0.99	0.13	57,57,57,57	0
2	IOD	A	201[B]	1/1	0.99	0.07	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.