



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:54 PM UTC

PDB ID : 2ZZD / pdb_00002zzd
Title : Recombinant thiocyanate hydrolase, air-oxidized form of holo-enzyme
Authors : Arakawa, T.; Kawano, Y.; Katayama, Y.; Yohda, M.; Odaka, M.
Deposited on : 2009-02-09
Resolution : 1.78 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

<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

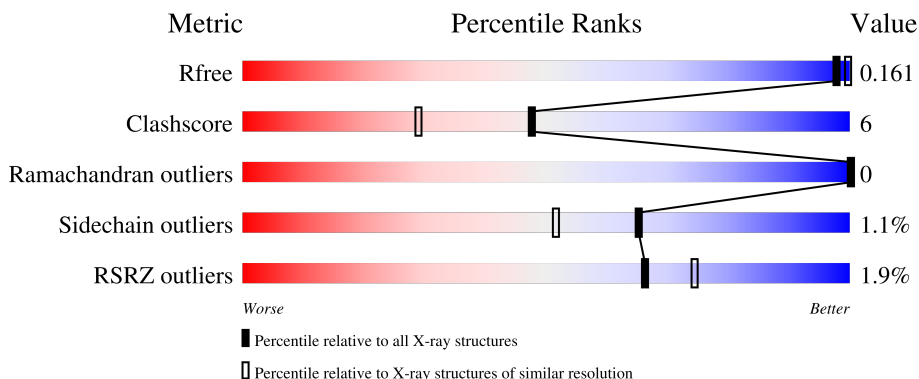
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	126	 3% 82% 12% • 6%
1	D	126	 2% 83% 10% • 5%
1	G	126	 3% 83% 12% • 5%
1	J	126	 2% 85% 10% 5%
2	B	157	 % 83% 12% • •

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Mol	Chain	Length	Quality of chain
2	E	157	<p>2% 83% 13% .</p>
2	H	157	<p>3% 87% 10% . .</p>
2	K	157	<p>% 86% 10% . .</p>
3	C	243	<p>% 81% 8% . 11%</p>
3	F	243	<p>2% 76% 12% . 10%</p>
3	I	243	<p>2% 77% 11% . 11%</p>
3	L	243	<p>% 78% 10% . 11%</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19243 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 Thiocyanate hydrolase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	119	Total 965	C 614	N 160	O 187	S 4	0	0	0
1	D	120	Total 974	C 620	N 162	O 188	S 4	0	0	0
1	G	120	Total 974	C 620	N 162	O 188	S 4	0	0	0
1	J	120	Total 974	C 620	N 162	O 188	S 4	0	0	0

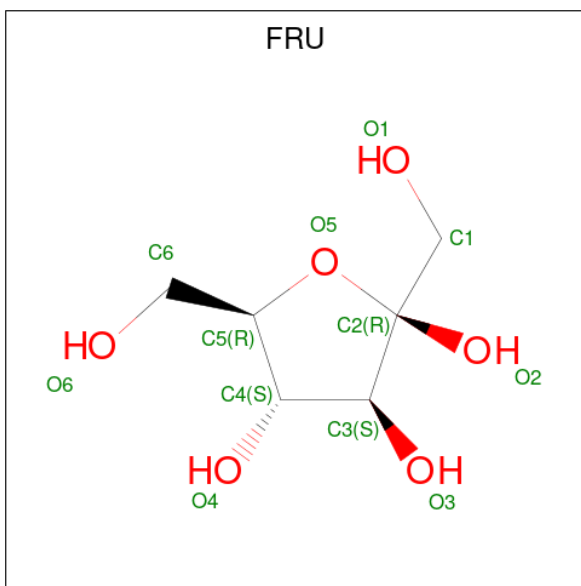
- Molecule 2 is a protein called Thiocyanate hydrolase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	153	Total 1241	C 784	N 224	O 227	S 6	0	0	0
2	E	151	Total 1226	C 775	N 221	O 224	S 6	0	0	0
2	H	156	Total 1262	C 796	N 228	O 232	S 6	0	0	0
2	K	152	Total 1232	C 778	N 222	O 226	S 6	0	0	0

- Molecule 3 is a protein called Thiocyanate hydrolase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	217	Total 1725	C 1098	N 304	O 315	S 8	0	0	0
3	F	218	Total 1735	C 1104	N 307	O 316	S 8	0	0	0
3	I	217	Total 1725	C 1098	N 304	O 315	S 8	0	0	0
3	L	216	Total 1716	C 1093	N 303	O 312	S 8	0	0	0

- Molecule 4 is beta-D-fructofuranose (CCD ID: FRU) (formula: C₆H₁₂O₆).

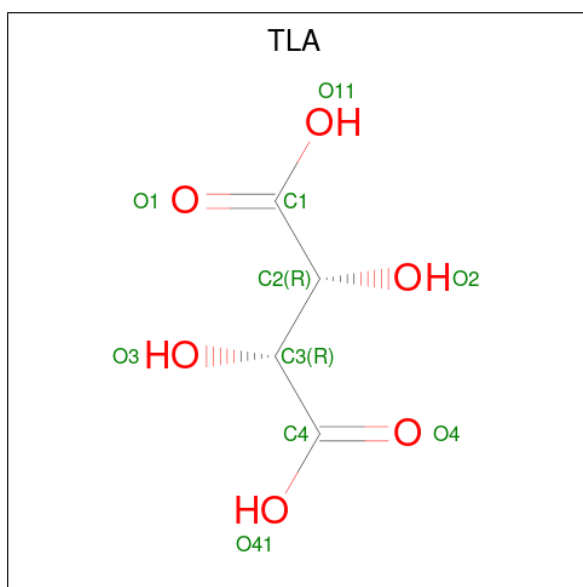


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 12 6 6	0	0
4	L	1	Total C O 12 6 6	0	0
4	L	1	Total C O 12 6 6	0	0

- Molecule 5 is COBALT (III) ION (CCD ID: 3CO) (formula: Co).

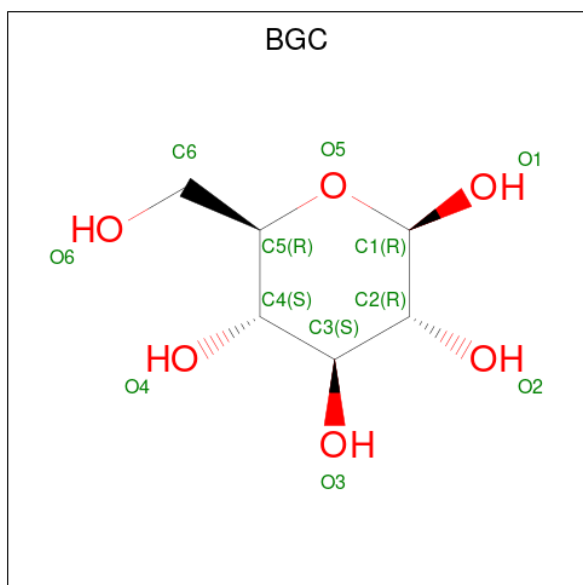
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Co 1 1	0	0
5	F	1	Total Co 1 1	0	0
5	I	1	Total Co 1 1	0	0
5	L	1	Total Co 1 1	0	0

- Molecule 6 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 10 4 6	0	0
6	F	1	Total C O 10 4 6	0	0
6	I	1	Total C O 10 4 6	0	0
6	L	1	Total C O 10 4 6	0	0

- Molecule 7 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			12	6	6		

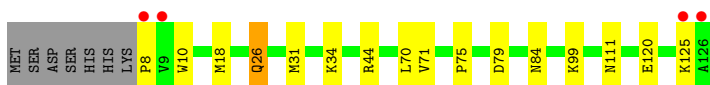
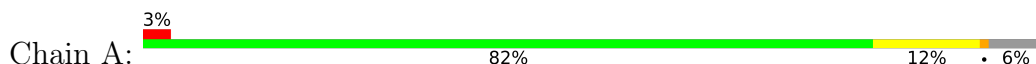
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	214	Total	O	0	0
			214	214		
8	B	265	Total	O	0	0
			265	265		
8	C	399	Total	O	0	0
			399	399		
8	D	216	Total	O	0	0
			216	216		
8	E	253	Total	O	0	0
			253	253		
8	F	352	Total	O	0	0
			352	352		
8	G	205	Total	O	0	0
			205	205		
8	H	260	Total	O	0	0
			260	260		
8	I	402	Total	O	0	0
			402	402		
8	J	206	Total	O	0	0
			206	206		
8	K	253	Total	O	0	0
			253	253		
8	L	377	Total	O	0	0
			377	377		

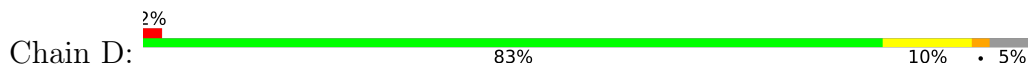
3 Residue-property plots [i](#)

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.

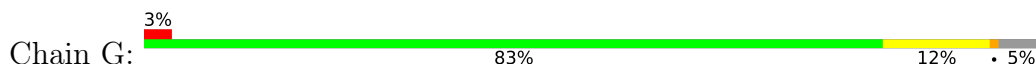
- Molecule 1: Thiocyanate hydrolase subunit alpha



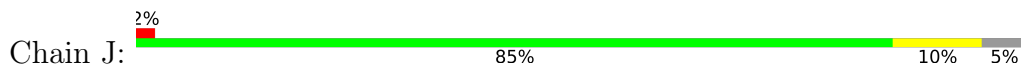
- Molecule 1: Thiocyanate hydrolase subunit alpha



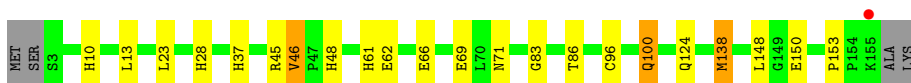
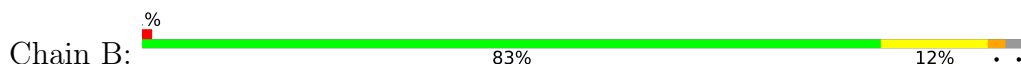
- Molecule 1: Thiocyanate hydrolase subunit alpha



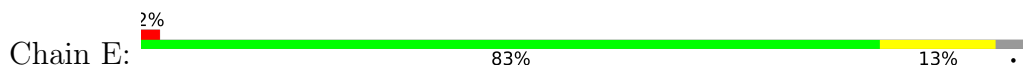
- Molecule 1: Thiocyanate hydrolase subunit alpha



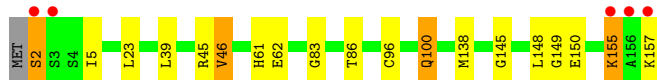
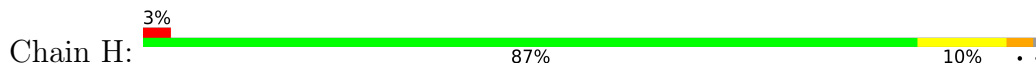
- Molecule 2: Thiocyanate hydrolase subunit beta



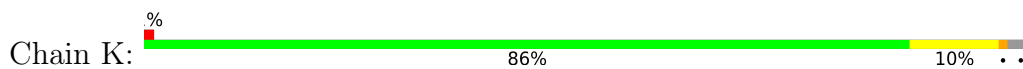
- Molecule 2: Thiocyanate hydrolase subunit beta



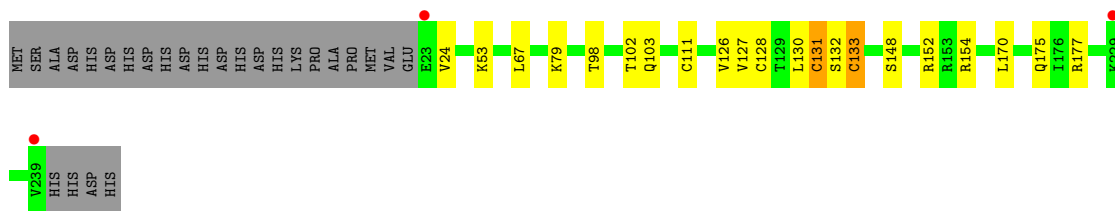
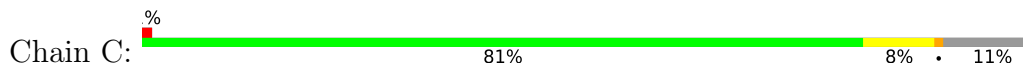
- Molecule 2: Thiocyanate hydrolase subunit beta



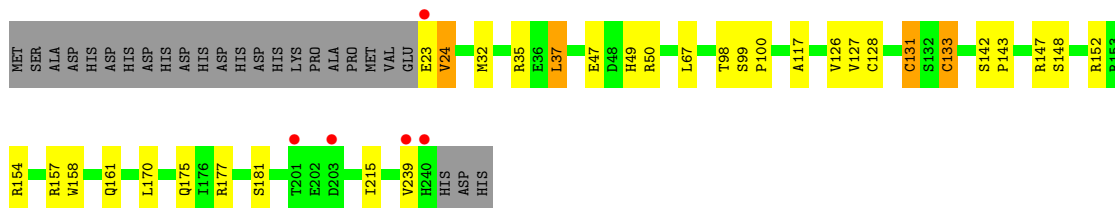
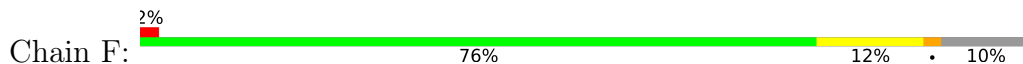
- Molecule 2: Thiocyanate hydrolase subunit beta



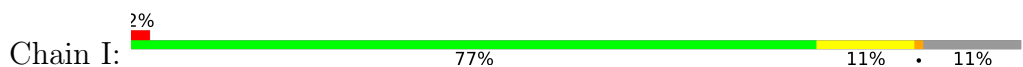
- Molecule 3: Thiocyanate hydrolase subunit gamma



- Molecule 3: Thiocyanate hydrolase subunit gamma



- Molecule 3: Thiocyanate hydrolase subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.01Å 170.76Å 175.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.76 – 1.78 40.76 – 1.78	Depositor EDS
% Data completeness (in resolution range)	94.3 (40.76-1.78) 97.3 (40.76-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 1.78Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.150 , 0.159 0.150 , 0.161	Depositor DCC
R_{free} test set	16106 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for -h,l,k	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19243	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: BGC, FRU, CSD, TLA, 3CO

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	0.35	0/991	0.98	4/1342 (0.3%)
1	D	0.36	0/1000	0.94	5/1354 (0.4%)
1	G	0.37	0/1000	0.95	4/1354 (0.3%)
1	J	0.36	0/1000	0.95	6/1354 (0.4%)
2	B	0.40	0/1273	0.93	6/1731 (0.3%)
2	E	0.37	0/1258	0.91	4/1712 (0.2%)
2	H	0.38	0/1294	0.95	7/1757 (0.4%)
2	K	0.38	0/1264	0.93	5/1720 (0.3%)
3	C	0.39	0/1753	0.93	4/2394 (0.2%)
3	F	0.41	0/1764	0.97	7/2409 (0.3%)
3	I	0.40	0/1753	0.94	6/2394 (0.3%)
3	L	0.40	0/1744	0.93	5/2382 (0.2%)
All	All	0.38	0/16094	0.94	63/21903 (0.3%)

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	154	ARG	N-CA-C	9.60	123.50	111.69
3	I	154	ARG	N-CA-C	9.46	123.33	111.69
3	F	154	ARG	N-CA-C	9.17	122.97	111.69
3	L	154	ARG	N-CA-C	9.10	122.89	111.69
2	H	46	VAL	N-CA-C	-8.87	99.49	107.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	965	0	914	20	0
1	D	974	0	926	13	0
1	G	974	0	926	14	0
1	J	974	0	926	9	0
2	B	1241	0	1211	28	0
2	E	1226	0	1193	19	0
2	H	1262	0	1234	15	0
2	K	1232	0	1198	15	0
3	C	1725	0	1735	12	0
3	F	1735	0	1742	24	0
3	I	1725	0	1735	16	0
3	L	1716	0	1729	17	0
4	B	12	0	12	5	0
4	L	24	0	24	2	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
6	C	10	0	4	0	0
6	F	10	0	4	0	0
6	I	10	0	4	0	0
6	L	10	0	4	0	0
7	F	12	0	12	0	0
8	A	214	0	0	8	0
8	B	265	0	0	3	0
8	C	399	0	0	3	0
8	D	216	0	0	7	0
8	E	253	0	0	10	0
8	F	352	0	0	5	0
8	G	205	0	0	5	0
8	H	260	0	0	5	0
8	I	402	0	0	2	0
8	J	206	0	0	5	0
8	K	253	0	0	5	0
8	L	377	0	0	5	0
All	All	19243	0	15533	175	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 175 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)
2:E:148:LEU:CD1	3:F:32:MET:HG3	1.87	1.04
1:A:26:GLN:HE21	1:A:26:GLN:H	1.11	0.98
8:G:3339:HOH:O	2:H:46:VAL:HG23	1.62	0.98
2:B:138:MET:HE3	2:B:138:MET:HA	1.45	0.96
2:E:148:LEU:HD11	3:F:32:MET:HG3	1.44	0.95

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	117/126 (93%)	113 (97%)	4 (3%)	0	100	100
1	D	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
1	G	118/126 (94%)	115 (98%)	3 (2%)	0	100	100
1	J	118/126 (94%)	115 (98%)	3 (2%)	0	100	100
2	B	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
2	E	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
2	H	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
2	K	150/157 (96%)	147 (98%)	3 (2%)	0	100	100
3	C	213/243 (88%)	206 (97%)	7 (3%)	0	100	100
3	F	214/243 (88%)	206 (96%)	8 (4%)	0	100	100
3	I	213/243 (88%)	205 (96%)	8 (4%)	0	100	100
3	L	212/243 (87%)	204 (96%)	8 (4%)	0	100	100
All	All	1927/2104 (92%)	1869 (97%)	58 (3%)	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	101/108 (94%)	99 (98%)	2 (2%)	48	29
1	D	102/108 (94%)	100 (98%)	2 (2%)	48	29
1	G	102/108 (94%)	100 (98%)	2 (2%)	48	29
1	J	102/108 (94%)	101 (99%)	1 (1%)	68	55
2	B	131/134 (98%)	130 (99%)	1 (1%)	73	63
2	E	129/134 (96%)	129 (100%)	0	100	100
2	H	133/134 (99%)	131 (98%)	2 (2%)	57	41
2	K	130/134 (97%)	130 (100%)	0	100	100
3	C	188/212 (89%)	186 (99%)	2 (1%)	65	51
3	F	189/212 (89%)	185 (98%)	4 (2%)	47	27
3	I	188/212 (89%)	187 (100%)	1 (0%)	81	73
3	L	187/212 (88%)	186 (100%)	1 (0%)	81	73
All	All	1682/1816 (93%)	1664 (99%)	18 (1%)	65	51

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	39	LEU
3	L	170	LEU
1	J	99	LYS
3	F	37	LEU
2	H	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	100	GLN

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Mol	Chain	Res	Type
2	K	124	GLN
2	E	94	GLN
2	E	61	HIS
3	L	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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
3	CSD	I	133	5,3	4,7,8	2.03	1 (25%)	1,8,10	1.93	0
3	CSD	F	131	5,3	4,7,8	2.29	1 (25%)	1,8,10	1.88	0
3	CSD	C	131	5,3	4,7,8	2.11	1 (25%)	1,8,10	1.95	0
3	CSD	L	133	5,3	4,7,8	2.29	1 (25%)	1,8,10	1.86	0
3	CSD	I	131	5,3	4,7,8	2.28	1 (25%)	1,8,10	1.83	0
3	CSD	C	133	5,3	4,7,8	2.38	1 (25%)	1,8,10	1.88	0
3	CSD	F	133	5,3	4,7,8	2.34	1 (25%)	1,8,10	1.86	0
3	CSD	L	131	5,3	4,7,8	2.36	1 (25%)	1,8,10	1.67	0

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	CSD	I	133	5,3	-	0/2/6/8	-
3	CSD	F	131	5,3	-	0/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CSD	C	131	5,3	-	0/2/6/8	-
3	CSD	L	133	5,3	-	0/2/6/8	-
3	CSD	I	131	5,3	-	0/2/6/8	-
3	CSD	C	133	5,3	-	0/2/6/8	-
3	CSD	F	133	5,3	-	0/2/6/8	-
3	CSD	L	131	5,3	-	0/2/6/8	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	131	CSD	OD1-SG	-4.52	1.43	1.47
3	C	133	CSD	OD1-SG	-4.48	1.43	1.47
3	F	133	CSD	OD1-SG	-4.41	1.43	1.47
3	F	131	CSD	OD1-SG	-4.37	1.43	1.47
3	L	133	CSD	OD1-SG	-4.35	1.43	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	133	CSD	1	0
3	F	131	CSD	1	0
3	C	131	CSD	1	0
3	L	133	CSD	1	0
3	I	131	CSD	1	0
3	C	133	CSD	1	0
3	F	133	CSD	1	0
3	L	131	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	FRU	L	6003	-	11,12,12	1.55	2 (18%)	10,18,18	1.68	2 (20%)
6	TLA	C	4001	-	9,9,9	1.05	0	12,12,12	1.05	1 (8%)
6	TLA	I	4003	-	9,9,9	1.08	0	12,12,12	1.03	1 (8%)
6	TLA	L	4004	-	9,9,9	1.02	0	12,12,12	1.03	1 (8%)
4	FRU	L	6001	-	11,12,12	1.55	4 (36%)	10,18,18	2.43	3 (30%)
4	FRU	B	6002	-	11,12,12	1.46	2 (18%)	10,18,18	1.65	1 (10%)
6	TLA	F	4002	-	9,9,9	1.05	0	12,12,12	1.02	1 (8%)
7	BGC	F	5001	-	12,12,12	0.38	0	17,17,17	0.36	0

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FRU	L	6003	-	-	1/5/24/24	0/1/1/1
6	TLA	C	4001	-	-	0/12/12/12	-
6	TLA	I	4003	-	-	0/12/12/12	-
6	TLA	L	4004	-	-	0/12/12/12	-
4	FRU	L	6001	-	-	2/5/24/24	0/1/1/1
4	FRU	B	6002	-	-	2/5/24/24	0/1/1/1
6	TLA	F	4002	-	-	0/12/12/12	-
7	BGC	F	5001	-	-	0/2/22/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	6002	FRU	C1-C2	3.41	1.60	1.52
4	L	6003	FRU	C1-C2	3.29	1.59	1.52
4	L	6003	FRU	O5-C5	3.22	1.50	1.43
4	L	6001	FRU	O2-C2	3.00	1.45	1.40
4	L	6001	FRU	C1-C2	2.55	1.58	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	6001	FRU	O2-C2-O5	6.15	121.13	109.33
4	B	6002	FRU	O2-C2-O5	4.19	117.37	109.33
4	L	6003	FRU	O2-C2-O5	3.17	115.42	109.33
4	L	6001	FRU	C6-C5-C4	2.92	122.00	115.10
4	L	6003	FRU	C6-C5-C4	-2.79	108.51	115.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	6002	FRU	O5-C5-C6-O6
4	B	6002	FRU	C4-C5-C6-O6
4	L	6001	FRU	C4-C5-C6-O6
4	L	6001	FRU	O5-C5-C6-O6
4	L	6003	FRU	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	6003	FRU	1	0
4	L	6001	FRU	1	0
4	B	6002	FRU	5	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	119/126 (94%)	-0.09	4 (3%) 48 55	11, 17, 32, 39	0
1	D	120/126 (95%)	-0.23	3 (2%) 58 66	11, 15, 31, 45	0
1	G	120/126 (95%)	-0.16	4 (3%) 49 56	11, 17, 31, 48	0
1	J	120/126 (95%)	-0.34	3 (2%) 58 66	10, 14, 28, 48	0
2	B	153/157 (97%)	-0.38	1 (0%) 84 88	10, 13, 26, 44	0
2	E	151/157 (96%)	-0.28	3 (1%) 65 73	10, 15, 32, 41	0
2	H	156/157 (99%)	-0.29	5 (3%) 50 57	10, 13, 26, 70	0
2	K	152/157 (96%)	-0.36	1 (0%) 84 88	10, 14, 29, 40	0
3	C	215/243 (88%)	-0.27	3 (1%) 73 80	10, 15, 26, 45	0
3	F	216/243 (88%)	0.02	5 (2%) 61 69	10, 18, 34, 54	0
3	I	215/243 (88%)	-0.34	4 (1%) 66 74	10, 14, 24, 46	0
3	L	214/243 (88%)	-0.32	2 (0%) 81 86	10, 14, 26, 36	0
All	All	1951/2104 (92%)	-0.25	38 (1%) 66 74	10, 15, 29, 70	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	156	ALA	8.1
2	H	2	SER	5.8
3	I	239	VAL	5.2
2	H	3	SER	5.0
3	F	240	HIS	4.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	CSD	I	133	8/9	0.97	0.06	11,12,15,15	1
3	CSD	C	133	8/9	0.98	0.06	11,13,15,16	1
3	CSD	F	131	8/9	0.98	0.06	12,12,13,14	0
3	CSD	F	133	8/9	0.98	0.06	12,14,15,15	1
3	CSD	C	131	8/9	0.98	0.06	10,12,13,15	0
3	CSD	L	133	8/9	0.98	0.07	10,11,14,14	1
3	CSD	L	131	8/9	0.99	0.05	10,11,12,12	0
3	CSD	I	131	8/9	0.99	0.04	11,12,13,14	0

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	FRU	B	6002	12/12	0.45	0.28	33,38,41,42	0
4	FRU	L	6001	12/12	0.62	0.27	43,51,59,60	0
4	FRU	L	6003	12/12	0.66	0.23	24,41,46,51	0
7	BGC	F	5001	12/12	0.92	0.08	25,27,28,28	0
6	TLA	I	4003	10/10	0.94	0.07	20,21,25,26	0
6	TLA	C	4001	10/10	0.96	0.07	19,20,24,26	0
6	TLA	F	4002	10/10	0.96	0.06	18,22,25,27	0
6	TLA	L	4004	10/10	0.97	0.06	16,18,23,24	0
5	3CO	F	301	1/1	1.00	0.01	14,14,14,14	0
5	3CO	I	301	1/1	1.00	0.03	14,14,14,14	0
5	3CO	L	301	1/1	1.00	0.02	13,13,13,13	0
5	3CO	C	301	1/1	1.00	0.01	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.