



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:01 PM GMT

PDB ID : 2DD4
Title : Thiocyanate hydrolase (SCNase) from Thiobacillus thioparus recombinant apo-enzyme
Authors : Arakawa, T.; Kawano, Y.; Kataoka, S.; Katayama, Y.; Kamiya, N.; Yohda, M.; Odaka, M.
Deposited on : 2006-01-19
Resolution : 2.06 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

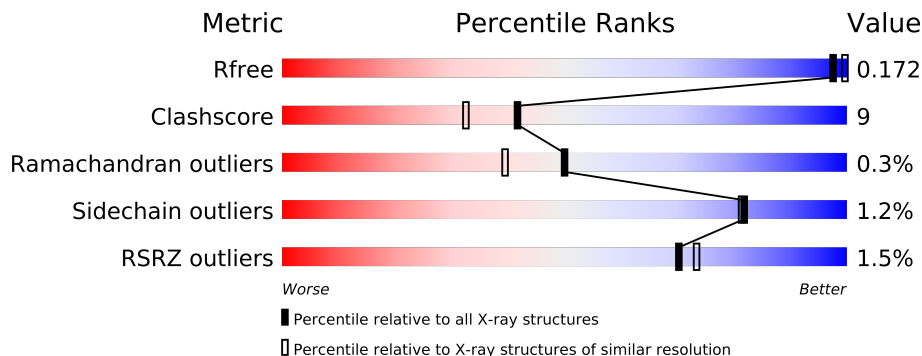
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.06 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}	66092	1224 (2.08-2.04)
Clashscore	79885	1390 (2.08-2.04)
Ramachandran outliers	78287	1381 (2.08-2.04)
Sidechain outliers	78261	1381 (2.08-2.04)
RSRZ outliers	66119	1225 (2.08-2.04)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	126	
1	D	126	
1	G	126	
1	J	126	
2	B	157	
2	E	157	
2	H	157	
2	K	157	
3	C	243	
3	F	243	
3	I	243	
3	L	243	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	FRU	B	3002	-	X
4	FRU	B	3008	-	X
4	FRU	C	3001	-	X
4	FRU	H	3004	-	X
4	FRU	H	3006	-	X
4	FRU	H	3007	-	X
4	FRU	K	3003	-	X
4	FRU	K	3005	-	X
5	TAR	C	3501	-	X
5	TAR	F	4501	-	X
5	TAR	I	5501	-	X
5	TAR	L	6501	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18077 atoms, of which 0 are hydrogen and 0 are deuterium.

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 alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			958	609	159	186	4			
1	D	119	Total	C	N	O	S	0	0	0
			965	614	160	187	4			
1	G	120	Total	C	N	O	S	0	0	0
			974	620	162	188	4			
1	J	120	Total	C	N	O	S	0	0	0
			974	620	162	188	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP O66187
D	1	MET	-	INITIATING METHIONINE	UNP O66187
G	1	MET	-	INITIATING METHIONINE	UNP O66187
J	1	MET	-	INITIATING METHIONINE	UNP O66187

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP O66186
E	1	MET	-	INITIATING METHIONINE	UNP O66186
H	1	MET	-	INITIATING METHIONINE	UNP O66186
K	1	MET	-	INITIATING METHIONINE	UNP O66186

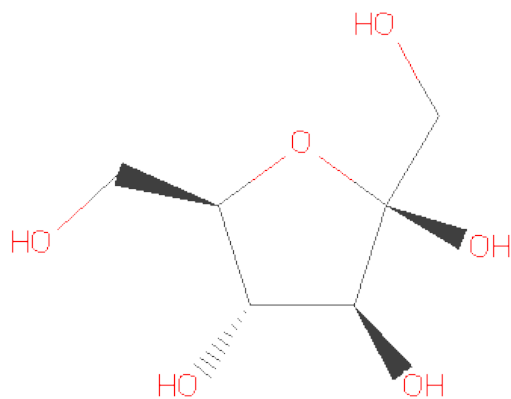
- Molecule 3 is a protein called Thiocyanate hydrolase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1721	1098	304	311	8			
3	F	216	Total	C	N	O	S	0	0	0
			1712	1093	303	308	8			
3	I	217	Total	C	N	O	S	0	0	0
			1721	1098	304	311	8			
3	L	216	Total	C	N	O	S	0	0	0
			1712	1093	303	308	8			

There are 4 discrepancies between the modelled and reference sequences:

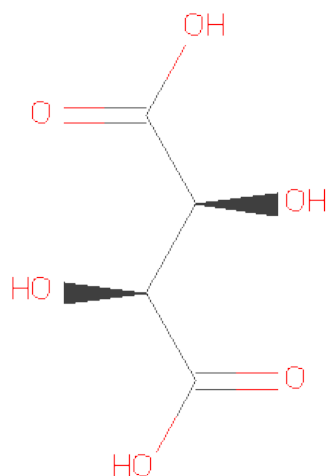
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	INITIATING METHIONINE	UNP O66188
F	1	MET	-	INITIATING METHIONINE	UNP O66188
I	1	MET	-	INITIATING METHIONINE	UNP O66188
L	1	MET	-	INITIATING METHIONINE	UNP O66188

- Molecule 4 is SUGAR (FRUCTOSE) (three-letter code: FRU) (formula: C₆H₁₂O₆).



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

- Molecule 5 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	182	Total	O	0	0
			182	182		
6	C	257	Total	O	0	0
			257	257		
6	D	123	Total	O	0	0
			123	123		
6	E	166	Total	O	0	0
			166	166		
6	F	209	Total	O	0	0
			209	209		
6	G	122	Total	O	0	0
			122	122		
6	H	185	Total	O	0	0
			185	185		
6	I	281	Total	O	0	0
			281	281		
6	J	132	Total	O	0	0
			132	132		
6	K	183	Total	O	0	0
			183	183		
6	L	252	Total	O	0	0
			252	252		

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 ($RSRZ > 2$). 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 alpha subunit

Chain A: 



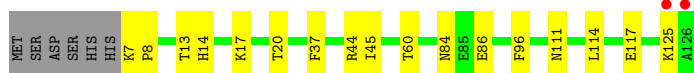
- Molecule 1: Thiocyanate hydrolase alpha subunit

Chain D: 



- Molecule 1: Thiocyanate hydrolase alpha subunit

Chain G: 



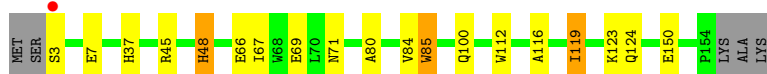
- Molecule 1: Thiocyanate hydrolase alpha subunit

Chain J: 



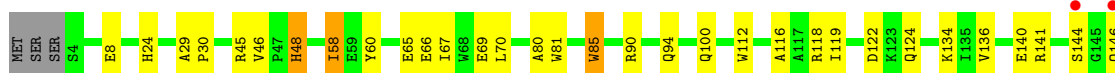
- Molecule 2: Thiocyanate hydrolase beta subunit

Chain B: 



- Molecule 2: Thiocyanate hydrolase beta subunit

Chain E: 



Y151	R152	R153	R154	R155	V156	R157	P158	P159	P160	Q161	E166	L170	P171	S172	E173	V174	Q175	I176	R177	V189	M190	P191	E207	I208	I215	P220	K221	I224	T225	V239	H15	H15	ASP	H15										
MET	SER	ALA	ASP	HIS	ASP	HIS	ASP	HIS	ASP	HIS	HIS	HIS	ASP	ASP	LYS	PRO	ALA	PRO	MET	VAL	GLU	GLU	V24	S25	D26	F27	E28	K32	D54	T58	L67	K78	I82	S99	P100	A117	K123	V127	C128	C131	Y134	S142	R147	M150

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	170.31Å 175.60Å 114.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.95 – 2.06 32.95 – 2.06	Depositor EDS
% Data completeness (in resolution range)	96.3 (32.95-2.06) 97.1 (32.95-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.56 (at 2.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.165 , 0.193 0.169 , 0.172	Depositor DCC
R_{free} test set	10298 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.5	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 204859 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18077	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.34	0/983	0.61	0/1331
1	D	0.33	0/991	0.60	0/1342
1	G	0.32	0/1000	0.59	0/1354
1	J	0.34	0/1000	0.60	0/1354
2	B	0.30	0/1264	0.58	0/1720
2	E	0.30	0/1258	0.57	0/1712
2	H	0.31	0/1294	0.58	0/1757
2	K	0.31	0/1264	0.59	0/1720
3	C	0.29	0/1765	0.60	0/2410
3	F	0.29	0/1756	0.60	0/2398
3	I	0.29	0/1765	0.61	0/2410
3	L	0.29	0/1756	0.61	0/2398
All	All	0.31	0/16096	0.60	0/21906

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	958	0	906	19	0
1	D	965	0	914	12	0
1	G	974	0	926	18	0
1	J	974	0	926	13	0
2	B	1232	0	1198	20	0
2	E	1226	0	1193	31	0
2	H	1262	0	1234	22	0
2	K	1232	0	1198	29	0
3	C	1721	0	1739	41	0
3	F	1712	0	1733	50	0
3	I	1721	0	1739	29	0
3	L	1712	0	1733	38	0
4	B	24	0	24	2	0
4	C	12	0	12	1	0
4	H	36	0	36	6	0
4	K	24	0	24	4	0
5	C	20	0	8	1	0
5	F	20	0	8	1	0
5	I	20	0	8	1	0
5	L	20	0	8	1	0
6	A	120	0	0	3	0
6	B	182	0	0	1	0
6	C	257	0	0	3	0
6	D	123	0	0	1	0
6	E	166	0	0	2	0
6	F	209	0	0	2	0
6	G	122	0	0	1	0
6	H	185	0	0	1	0
6	I	281	0	0	2	0
6	J	132	0	0	2	0
6	K	183	0	0	0	0
6	L	252	0	0	2	0
All	All	18077	0	15567	287	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 287 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:113:LEU:HD11	3:F:188:ILE:HD12	1.36	1.05
3:I:82:ILE:HD11	3:I:117:ALA:HB2	1.44	1.00
1:A:26:GLN:HE21	1:A:26:GLN:H	1.08	0.97
3:F:115:VAL:HG22	3:F:188:ILE:HD11	1.47	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:45:ILE:HD11	1:D:96:PHE:HZ	1.32	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	116/126 (92%)	109 (94%)	7 (6%)	0	100	100
1	D	117/126 (93%)	111 (95%)	6 (5%)	0	100	100
1	G	118/126 (94%)	115 (98%)	3 (2%)	0	100	100
1	J	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
2	B	150/157 (96%)	147 (98%)	3 (2%)	0	100	100
2	E	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
2	H	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
2	K	150/157 (96%)	146 (97%)	4 (3%)	0	100	100
3	C	215/243 (88%)	206 (96%)	8 (4%)	1 (0%)	38	25
3	F	214/243 (88%)	205 (96%)	7 (3%)	2 (1%)	25	11
3	I	215/243 (88%)	206 (96%)	8 (4%)	1 (0%)	38	25
3	L	214/243 (88%)	205 (96%)	8 (4%)	1 (0%)	38	25
All	All	1930/2104 (92%)	1859 (96%)	66 (3%)	5 (0%)	50	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	131	CYS
3	F	131	CYS
3	I	131	CYS
3	L	131	CYS
3	F	238	PRO

5.3.2 Protein sidechains ⓘ

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	100/108 (93%)	98 (98%)	2 (2%)	68	65
1	D	101/108 (94%)	101 (100%)	0	100	100
1	G	102/108 (94%)	102 (100%)	0	100	100
1	J	102/108 (94%)	102 (100%)	0	100	100
2	B	130/134 (97%)	127 (98%)	3 (2%)	63	58
2	E	129/134 (96%)	126 (98%)	3 (2%)	63	58
2	H	133/134 (99%)	129 (97%)	4 (3%)	53	46
2	K	130/134 (97%)	127 (98%)	3 (2%)	63	58
3	C	190/214 (89%)	190 (100%)	0	100	100
3	F	189/214 (88%)	186 (98%)	3 (2%)	75	73
3	I	190/214 (89%)	189 (100%)	1 (0%)	94	94
3	L	189/214 (88%)	188 (100%)	1 (0%)	94	94
All	All	1685/1824 (92%)	1665 (99%)	20 (1%)	82	81

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	37	LEU
3	F	188	ILE
2	K	48	HIS
2	E	85	TRP
3	F	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	175	GLN
1	G	84	ASN
2	K	100	GLN
1	G	14	HIS
2	H	61	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 ligands 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$
4	FRU	B	3002	-	12,12,12	1.26	2 (16%)	18,18,18	2.89	5 (27%)
4	FRU	B	3008	-	12,12,12	2.41	5 (41%)	18,18,18	7.96	11 (61%)
4	FRU	C	3001	-	12,12,12	1.49	2 (16%)	18,18,18	2.91	5 (27%)
5	TAR	C	3401	-	9,9,9	1.19	1 (11%)	12,12,12	0.89	0
5	TAR	C	3501	-	9,9,9	1.16	1 (11%)	12,12,12	0.88	0
5	TAR	F	4401	-	9,9,9	1.17	1 (11%)	12,12,12	0.86	0
5	TAR	F	4501	-	9,9,9	1.07	1 (11%)	12,12,12	0.84	0
4	FRU	H	3004	-	12,12,12	1.33	2 (16%)	18,18,18	2.95	6 (33%)
4	FRU	H	3006	-	12,12,12	1.25	1 (8%)	18,18,18	3.06	6 (33%)
4	FRU	H	3007	-	12,12,12	1.57	2 (16%)	18,18,18	2.89	5 (27%)
5	TAR	I	5401	-	9,9,9	1.28	1 (11%)	12,12,12	0.85	0
5	TAR	I	5501	-	9,9,9	1.24	1 (11%)	12,12,12	0.87	0
4	FRU	K	3003	-	12,12,12	1.32	2 (16%)	18,18,18	2.92	6 (33%)
4	FRU	K	3005	-	12,12,12	1.48	2 (16%)	18,18,18	2.91	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	TAR	L	6401	-	9,9,9	1.17	1 (11%)	12,12,12	0.81	0
5	TAR	L	6501	-	9,9,9	1.22	1 (11%)	12,12,12	0.91	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
4	FRU	B	3002	-	-	0/5/24/24	0/1/1/1
4	FRU	B	3008	-	-	0/5/24/24	0/1/1/1
4	FRU	C	3001	-	-	0/5/24/24	0/1/1/1
5	TAR	C	3401	-	2/2/4/4	0/12/12/12	0/0/0/0
5	TAR	C	3501	-	2/2/4/4	0/12/12/12	0/0/0/0
5	TAR	F	4401	-	2/2/4/4	0/12/12/12	0/0/0/0
5	TAR	F	4501	-	2/2/4/4	0/12/12/12	0/0/0/0
4	FRU	H	3004	-	-	0/5/24/24	0/1/1/1
4	FRU	H	3006	-	-	0/5/24/24	0/1/1/1
4	FRU	H	3007	-	-	0/5/24/24	0/1/1/1
5	TAR	I	5401	-	2/2/4/4	0/12/12/12	0/0/0/0
5	TAR	I	5501	-	2/2/4/4	0/12/12/12	0/0/0/0
4	FRU	K	3003	-	-	0/5/24/24	0/1/1/1
4	FRU	K	3005	-	-	0/5/24/24	0/1/1/1
5	TAR	L	6401	-	2/2/4/4	0/12/12/12	0/0/0/0
5	TAR	L	6501	-	2/2/4/4	0/12/12/12	0/0/0/0

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3008	FRU	C1-C2	4.89	1.60	1.52
4	H	3007	FRU	C1-C2	4.26	1.59	1.52
4	C	3001	FRU	C1-C2	4.12	1.59	1.52
4	K	3005	FRU	C1-C2	4.08	1.59	1.52
4	B	3008	FRU	C2-C3	3.61	1.63	1.53

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3008	FRU	O2-C2-O5	-15.96	76.33	109.47
4	B	3008	FRU	O2-C2-C3	13.52	139.37	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3008	FRU	O2-C2-C1	-13.44	73.78	108.41
4	B	3008	FRU	O5-C2-C3	-12.76	78.14	104.82
4	B	3008	FRU	O5-C2-C1	12.63	128.06	108.17

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	4501	TAR	C2
5	F	4501	TAR	C3
5	C	3501	TAR	C2
5	C	3501	TAR	C3
5	C	3401	TAR	C2

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	118/126 (93%)	-0.34	1 (0%) 83 86	8, 14, 28, 34	0
1	D	119/126 (94%)	-0.34	1 (0%) 83 86	8, 13, 29, 36	0
1	G	120/126 (95%)	-0.30	2 (1%) 67 70	9, 15, 29, 43	0
1	J	120/126 (95%)	-0.43	2 (1%) 67 70	7, 12, 29, 38	0
2	B	152/157 (96%)	-0.55	1 (0%) 84 88	7, 11, 24, 33	0
2	E	151/157 (96%)	-0.48	4 (2%) 53 55	6, 12, 31, 41	0
2	H	156/157 (99%)	-0.46	4 (2%) 53 55	7, 11, 23, 60	0
2	K	152/157 (96%)	-0.49	4 (2%) 53 55	5, 11, 29, 37	0
3	C	217/243 (89%)	-0.38	2 (0%) 81 83	7, 14, 25, 46	0
3	F	216/243 (88%)	-0.12	5 (2%) 57 59	7, 16, 30, 43	0
3	I	217/243 (89%)	-0.47	2 (0%) 81 83	8, 12, 21, 42	0
3	L	216/243 (88%)	-0.41	1 (0%) 88 92	7, 11, 23, 34	0
All	All	1954/2104 (92%)	-0.39	29 (1%) 70 73	5, 13, 27, 60	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	157	LYS	7.8
3	F	239	VAL	7.7
2	H	156	ALA	7.2
2	H	2	SER	4.5
2	H	3	SER	4.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	FRU	H	3004	12/12	0.29	27.81	29,37,41,42	0
4	FRU	H	3007	12/12	0.37	15.40	35,38,40,40	0
4	FRU	H	3006	12/12	0.38	14.45	39,45,48,49	0
4	FRU	C	3001	12/12	0.27	12.37	32,36,37,41	0
4	FRU	B	3002	12/12	0.30	11.29	29,37,40,40	0
4	FRU	B	3008	12/12	0.32	10.06	32,37,40,41	0
4	FRU	K	3005	12/12	0.28	9.34	29,34,36,39	0
5	TAR	I	5501	10/10	0.21	8.14	20,24,28,30	0
5	TAR	F	4501	10/10	0.16	7.70	18,23,27,29	0
5	TAR	C	3501	10/10	0.16	7.22	16,22,29,29	0
4	FRU	K	3003	12/12	0.32	6.85	43,45,49,50	0
5	TAR	L	6501	10/10	0.13	6.26	15,21,26,28	0
5	TAR	L	6401	10/10	0.11	1.01	13,15,19,19	0
5	TAR	I	5401	10/10	0.11	0.33	13,16,19,21	0
5	TAR	C	3401	10/10	0.10	-0.15	14,17,19,22	0
5	TAR	F	4401	10/10	0.09	-0.74	13,16,18,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.