



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID : 2Q4S
Title : Ensemble refinement of the protein crystal structure of cysteine dioxygenase type I from *Mus musculus* Mm.241056
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 1.75 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

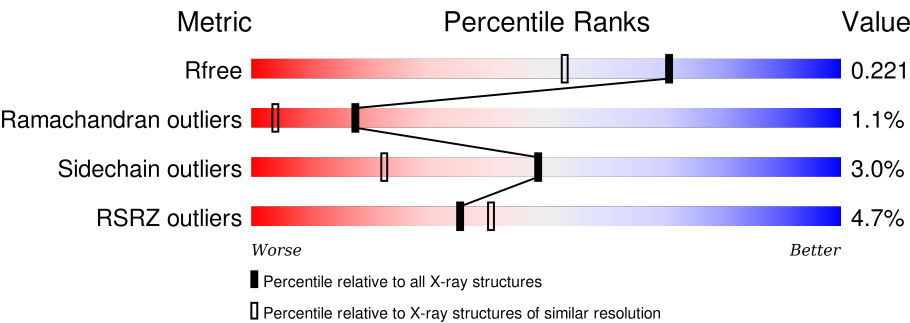
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





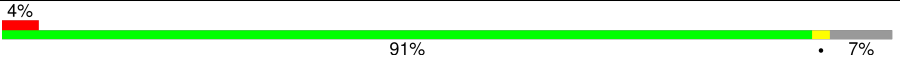
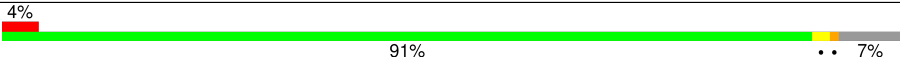
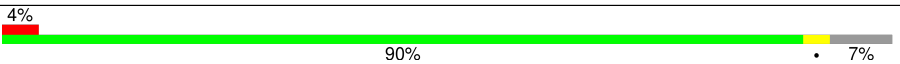
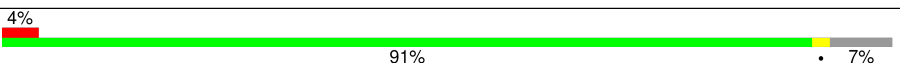
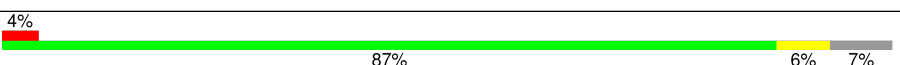
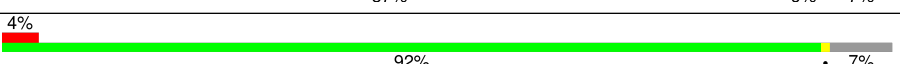
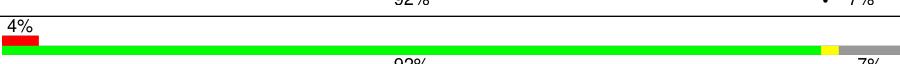
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1609 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	200	<div><div>4%</div><div>90%</div><div>7%</div></div>
1	10-A	200	<div><div>4%</div><div>88%</div><div>7%</div></div>
1	11-A	200	<div><div>4%</div><div>91%</div><div>7%</div></div>
1	12-A	200	<div><div>4%</div><div>90%</div><div>7%</div></div>
1	13-A	200	<div><div>4%</div><div>83%</div><div>10%</div><div>7%</div></div>
1	14-A	200	<div><div>4%</div><div>88%</div><div>5%</div><div>7%</div></div>
1	15-A	200	<div><div>4%</div><div>87%</div><div>5%</div><div>7%</div></div>

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Mol	Chain	Length	Quality of chain
1	16-A	200	
1	2-A	200	
1	3-A	200	
1	4-A	200	
1	5-A	200	
1	6-A	200	
1	7-A	200	
1	8-A	200	
1	9-A	200	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27280 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 Cysteine dioxygenase type 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	2-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	3-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	4-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	5-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	6-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	7-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	8-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	9-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	10-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	11-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	12-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	13-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	14-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	15-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			
1	16-A	186	Total	C	N	O	S	Se	0	0	0
			1512	955	267	283	4	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP P60334
A	73	MSE	MET	MODIFIED RESIDUE	UNP P60334
A	117	MSE	MET	MODIFIED RESIDUE	UNP P60334
A	179	MSE	MET	MODIFIED RESIDUE	UNP P60334

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	3-A	1	Total Ni 1 1	0	0
2	11-A	1	Total Ni 1 1	0	0
2	16-A	1	Total Ni 1 1	0	0
2	4-A	1	Total Ni 1 1	0	0
2	12-A	1	Total Ni 1 1	0	0
2	5-A	1	Total Ni 1 1	0	0
2	13-A	1	Total Ni 1 1	0	0
2	8-A	1	Total Ni 1 1	0	0
2	1-A	1	Total Ni 1 1	0	0
2	6-A	1	Total Ni 1 1	0	0
2	14-A	1	Total Ni 1 1	0	0
2	2-A	1	Total Ni 1 1	0	0
2	10-A	1	Total Ni 1 1	0	0
2	9-A	1	Total Ni 1 1	0	0
2	7-A	1	Total Ni 1 1	0	0
2	15-A	1	Total Ni 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	O	0	0
			4	2	2		
3	2-A	1	Total	C	O	0	0
			4	2	2		
3	3-A	1	Total	C	O	0	0
			4	2	2		
3	4-A	1	Total	C	O	0	0
			4	2	2		
3	5-A	1	Total	C	O	0	0
			4	2	2		
3	6-A	1	Total	C	O	0	0
			4	2	2		
3	7-A	1	Total	C	O	0	0
			4	2	2		
3	8-A	1	Total	C	O	0	0
			4	2	2		
3	9-A	1	Total	C	O	0	0
			4	2	2		
3	10-A	1	Total	C	O	0	0
			4	2	2		
3	11-A	1	Total	C	O	0	0
			4	2	2		
3	12-A	1	Total	C	O	0	0
			4	2	2		
3	13-A	1	Total	C	O	0	0
			4	2	2		
3	14-A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	15-A	1	Total	C	O	0	0
			4	2	2		
3	16-A	1	Total	C	O	0	0
			4	2	2		

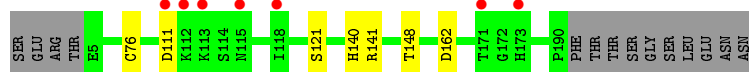
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	188	Total	O	0	0
			188	188		
4	2-A	188	Total	O	0	0
			188	188		
4	3-A	188	Total	O	0	0
			188	188		
4	4-A	188	Total	O	0	0
			188	188		
4	5-A	188	Total	O	0	0
			188	188		
4	6-A	188	Total	O	0	0
			188	188		
4	7-A	188	Total	O	0	0
			188	188		
4	8-A	188	Total	O	0	0
			188	188		
4	9-A	188	Total	O	0	0
			188	188		
4	10-A	188	Total	O	0	0
			188	188		
4	11-A	188	Total	O	0	0
			188	188		
4	12-A	188	Total	O	0	0
			188	188		
4	13-A	188	Total	O	0	0
			188	188		
4	14-A	188	Total	O	0	0
			188	188		
4	15-A	188	Total	O	0	0
			188	188		
4	16-A	188	Total	O	0	0
			188	188		

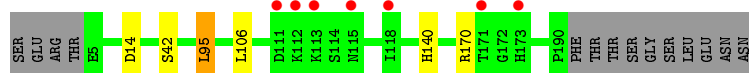
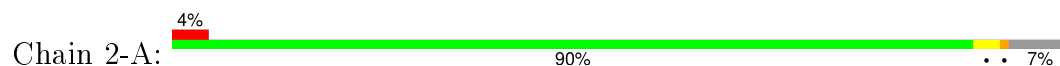
3 Residue-property plots [i](#)

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.

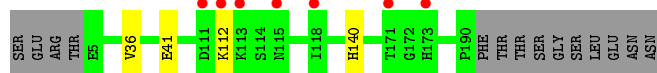
- Molecule 1: Cysteine dioxygenase type 1



- Molecule 1: Cysteine dioxygenase type 1



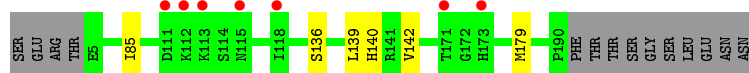
- Molecule 1: Cysteine dioxygenase type 1



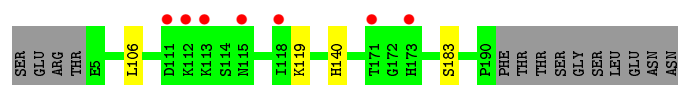
- Molecule 1: Cysteine dioxygenase type 1



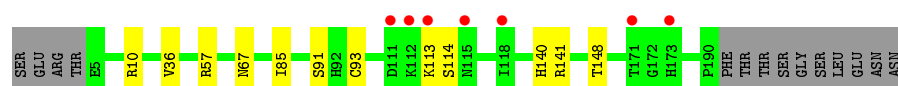
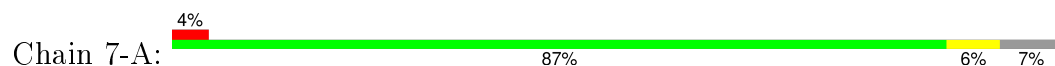
- Molecule 1: Cysteine dioxygenase type 1



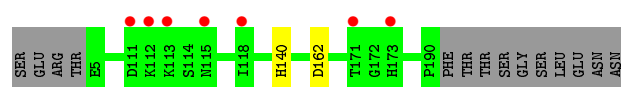
- Molecule 1: Cysteine dioxygenase type 1



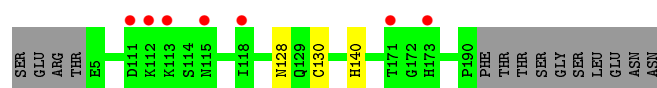
- Molecule 1: Cysteine dioxygenase type 1



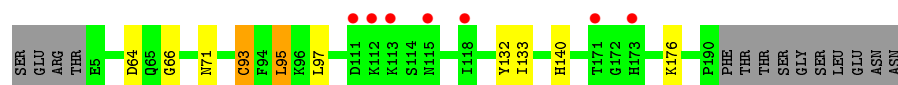
- Molecule 1: Cysteine dioxygenase type 1



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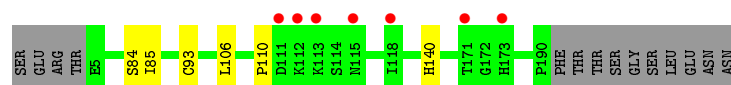
- Molecule 1: Cysteine dioxygenase type 1



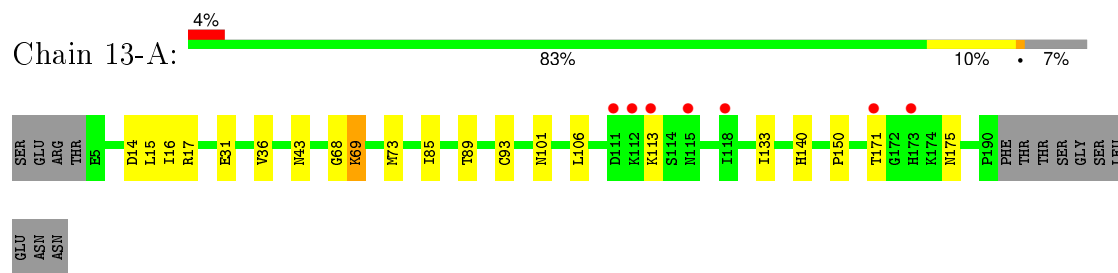
- Molecule 1: Cysteine dioxygenase type 1



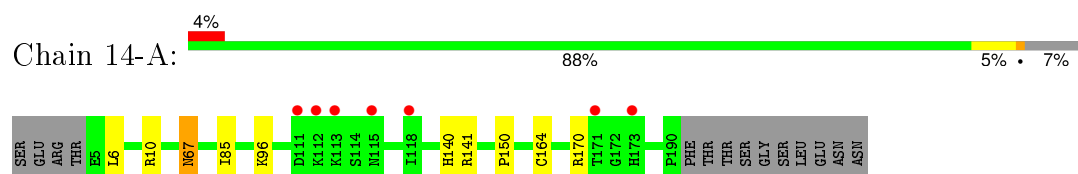
- Molecule 1: Cysteine dioxygenase type 1



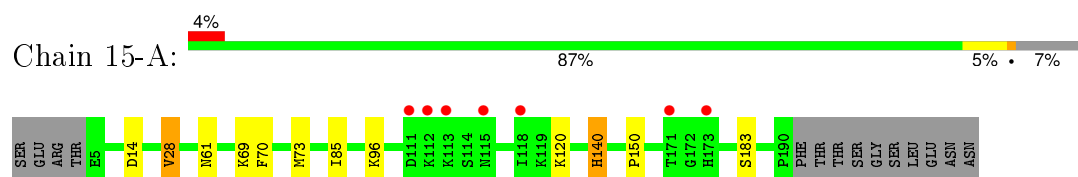
- Molecule 1: Cysteine dioxygenase type 1



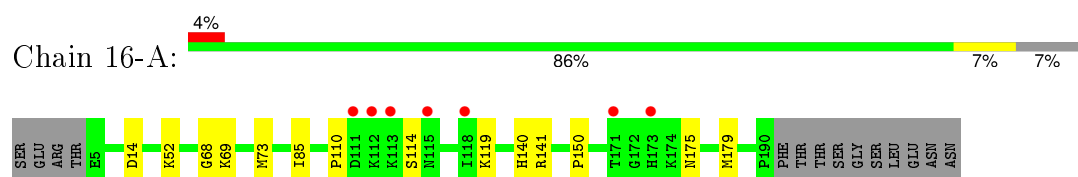
- Molecule 1: Cysteine dioxygenase type 1



- Molecule 1: Cysteine dioxygenase type 1



- Molecule 1: Cysteine dioxygenase type 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	57.55Å 57.55Å 122.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.86 – 1.75 33.86 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.86-1.75) 100.0 (33.86-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.14 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.159 , 0.211 0.169 , 0.221	Depositor DCC
R_{free} test set	1101 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21463 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27280	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1-A	0.73	0/1547	0.82	1/2088 (0.0%)
1	2-A	0.70	0/1547	0.82	2/2088 (0.1%)
1	3-A	0.70	0/1547	0.77	0/2088
1	4-A	0.68	0/1547	0.82	1/2088 (0.0%)
1	5-A	0.68	0/1547	0.80	0/2088
1	6-A	0.71	0/1547	0.79	1/2088 (0.0%)
1	7-A	0.74	0/1547	0.82	2/2088 (0.1%)
1	8-A	0.71	0/1547	0.77	0/2088
1	9-A	0.74	1/1547 (0.1%)	0.76	0/2088
1	10-A	0.87	1/1547 (0.1%)	0.86	1/2088 (0.0%)
1	11-A	0.68	0/1547	0.79	2/2088 (0.1%)
1	12-A	0.74	1/1547 (0.1%)	0.81	1/2088 (0.0%)
1	13-A	0.84	2/1547 (0.1%)	0.91	1/2088 (0.0%)
1	14-A	0.82	0/1547	0.89	1/2088 (0.0%)
1	15-A	0.86	0/1547	0.90	1/2088 (0.0%)
1	16-A	0.85	0/1547	0.93	3/2088 (0.1%)
All	All	0.76	5/24752 (0.0%)	0.83	17/33408 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	93	CYS	CB-SG	18.29	2.13	1.82
1	12-A	93	CYS	CB-SG	9.18	1.97	1.82
1	9-A	130	CYS	CB-SG	6.58	1.93	1.82
1	13-A	31	GLU	CD-OE2	-5.78	1.19	1.25
1	13-A	93	CYS	CB-SG	-5.30	1.73	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	95	LEU	CA-CB-CG	6.73	130.78	115.30
1	14-A	85	ILE	N-CA-C	-6.43	93.64	111.00
1	2-A	95	LEU	CA-CB-CG	6.31	129.82	115.30
1	13-A	85	ILE	N-CA-C	-6.02	94.75	111.00
1	12-A	106	LEU	CA-CB-CG	5.83	128.71	115.30
1	2-A	106	LEU	CA-CB-CG	5.74	128.51	115.30
1	6-A	106	LEU	CA-CB-CG	5.74	128.49	115.30
1	1-A	141	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	11-A	85	ILE	N-CA-C	-5.64	95.76	111.00
1	16-A	85	ILE	N-CA-C	-5.48	96.20	111.00
1	4-A	95	LEU	CA-CB-CG	5.47	127.89	115.30
1	7-A	141	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	16-A	52	LYS	CD-CE-NZ	5.42	124.17	111.70
1	11-A	130	CYS	CA-CB-SG	5.40	123.72	114.00
1	7-A	85	ILE	N-CA-C	-5.25	96.82	111.00
1	16-A	68	GLY	N-CA-C	5.13	125.92	113.10
1	15-A	85	ILE	N-CA-C	-5.11	97.20	111.00

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	1-A	1512	0	1459	0	0
1	2-A	1512	0	1459	0	0
1	3-A	1512	0	1459	0	0
1	4-A	1512	0	1459	0	0
1	5-A	1512	0	1459	0	0
1	6-A	1512	0	1459	0	0
1	7-A	1512	0	1459	0	0
1	8-A	1512	0	1459	0	0
1	9-A	1512	0	1459	0	0
1	10-A	1512	0	1459	0	0
1	11-A	1512	0	1459	0	0
1	12-A	1512	0	1459	0	0
1	13-A	1512	0	1459	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	14-A	1512	0	1459	0	0
1	15-A	1512	0	1459	0	0
1	16-A	1512	0	1459	0	0
2	1-A	1	0	0	0	0
2	2-A	1	0	0	0	0
2	3-A	1	0	0	0	0
2	4-A	1	0	0	0	0
2	5-A	1	0	0	0	0
2	6-A	1	0	0	0	0
2	7-A	1	0	0	0	0
2	8-A	1	0	0	0	0
2	9-A	1	0	0	0	0
2	10-A	1	0	0	0	0
2	11-A	1	0	0	0	0
2	12-A	1	0	0	0	0
2	13-A	1	0	0	0	0
2	14-A	1	0	0	0	0
2	15-A	1	0	0	0	0
2	16-A	1	0	0	0	0
3	1-A	4	0	6	0	0
3	2-A	4	0	6	0	0
3	3-A	4	0	6	0	0
3	4-A	4	0	6	0	0
3	5-A	4	0	6	0	0
3	6-A	4	0	6	0	0
3	7-A	4	0	6	0	0
3	8-A	4	0	6	0	0
3	9-A	4	0	6	0	0
3	10-A	4	0	6	0	0
3	11-A	4	0	6	0	0
3	12-A	4	0	6	0	0
3	13-A	4	0	6	0	0
3	14-A	4	0	6	0	0
3	15-A	4	0	6	0	0
3	16-A	4	0	6	0	0
4	1-A	188	0	0	0	0
4	2-A	188	0	0	0	0
4	3-A	188	0	0	0	0
4	4-A	188	0	0	0	0
4	5-A	188	0	0	0	0
4	6-A	188	0	0	0	0
4	7-A	188	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	8-A	188	0	0	0	0
4	9-A	188	0	0	0	0
4	10-A	188	0	0	0	0
4	11-A	188	0	0	0	0
4	12-A	188	0	0	0	0
4	13-A	188	0	0	0	0
4	14-A	188	0	0	0	0
4	15-A	188	0	0	0	0
4	16-A	188	0	0	0	0
All	All	27280	0	23440	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	184/200 (92%)	173 (94%)	9 (5%)	2 (1%)	17	4
1	2-A	184/200 (92%)	175 (95%)	8 (4%)	1 (0%)	34	14
1	3-A	184/200 (92%)	179 (97%)	4 (2%)	1 (0%)	34	14
1	4-A	184/200 (92%)	180 (98%)	3 (2%)	1 (0%)	34	14
1	5-A	184/200 (92%)	173 (94%)	9 (5%)	2 (1%)	17	4
1	6-A	184/200 (92%)	179 (97%)	5 (3%)	0	100	100
1	7-A	184/200 (92%)	166 (90%)	13 (7%)	5 (3%)	6	0
1	8-A	184/200 (92%)	182 (99%)	2 (1%)	0	100	100
1	9-A	184/200 (92%)	181 (98%)	2 (1%)	1 (0%)	34	14
1	10-A	184/200 (92%)	168 (91%)	12 (6%)	4 (2%)	8	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11-A	184/200 (92%)	180 (98%)	3 (2%)	1 (0%)	34	14
1	12-A	184/200 (92%)	176 (96%)	6 (3%)	2 (1%)	17	4
1	13-A	184/200 (92%)	168 (91%)	10 (5%)	6 (3%)	5	0
1	14-A	184/200 (92%)	175 (95%)	8 (4%)	1 (0%)	34	14
1	15-A	184/200 (92%)	172 (94%)	9 (5%)	3 (2%)	12	2
1	16-A	184/200 (92%)	176 (96%)	6 (3%)	2 (1%)	17	4
All	All	2944/3200 (92%)	2803 (95%)	109 (4%)	32 (1%)	17	4

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	5-A	142	VAL
1	7-A	113	LYS
1	7-A	114	SER
1	10-A	133	ILE
1	12-A	85	ILE
1	13-A	15	LEU
1	13-A	69	LYS
1	13-A	113	LYS
1	1-A	111	ASP
1	3-A	112	LYS
1	5-A	85	ILE
1	7-A	57	ARG
1	10-A	132	TYR
1	13-A	16	ILE
1	13-A	68	GLY
1	14-A	67	ASN
1	16-A	119	LYS
1	7-A	10	ARG
1	9-A	128	ASN
1	10-A	176	LYS
1	15-A	140	HIS
1	15-A	183	SER
1	1-A	121	SER
1	11-A	137	ILE
1	16-A	114	SER
1	2-A	42	SER
1	7-A	67	ASN
1	13-A	89	THR
1	10-A	66	GLY

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Mol	Chain	Res	Type
1	12-A	110	PRO
1	15-A	28	VAL
1	4-A	110	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	1-A	166/176 (94%)	162 (98%)	4 (2%)	57	31
1	2-A	166/176 (94%)	162 (98%)	4 (2%)	57	31
1	3-A	166/176 (94%)	163 (98%)	3 (2%)	66	46
1	4-A	166/176 (94%)	163 (98%)	3 (2%)	66	46
1	5-A	166/176 (94%)	162 (98%)	4 (2%)	57	31
1	6-A	166/176 (94%)	163 (98%)	3 (2%)	66	46
1	7-A	166/176 (94%)	161 (97%)	5 (3%)	48	22
1	8-A	166/176 (94%)	164 (99%)	2 (1%)	78	62
1	9-A	166/176 (94%)	165 (99%)	1 (1%)	90	83
1	10-A	166/176 (94%)	160 (96%)	6 (4%)	42	16
1	11-A	166/176 (94%)	165 (99%)	1 (1%)	90	83
1	12-A	166/176 (94%)	164 (99%)	2 (1%)	78	62
1	13-A	166/176 (94%)	153 (92%)	13 (8%)	16	2
1	14-A	166/176 (94%)	157 (95%)	9 (5%)	27	7
1	15-A	166/176 (94%)	156 (94%)	10 (6%)	24	5
1	16-A	166/176 (94%)	157 (95%)	9 (5%)	27	7
All	All	2656/2816 (94%)	2577 (97%)	79 (3%)	48	22

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	76	CYS

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Mol	Chain	Res	Type
1	1-A	140	HIS
1	1-A	148	THR
1	1-A	162	ASP
1	2-A	14	ASP
1	2-A	95	LEU
1	2-A	140	HIS
1	2-A	170	ARG
1	3-A	36	VAL
1	3-A	41	GLU
1	3-A	140	HIS
1	4-A	95	LEU
1	4-A	140	HIS
1	4-A	162	ASP
1	5-A	136	SER
1	5-A	139	LEU
1	5-A	140	HIS
1	5-A	179	MSE
1	6-A	119	LYS
1	6-A	140	HIS
1	6-A	183	SER
1	7-A	36	VAL
1	7-A	91	SER
1	7-A	93	CYS
1	7-A	140	HIS
1	7-A	148	THR
1	8-A	140	HIS
1	8-A	162	ASP
1	9-A	140	HIS
1	10-A	64	ASP
1	10-A	71	ASN
1	10-A	93	CYS
1	10-A	95	LEU
1	10-A	97	LEU
1	10-A	140	HIS
1	11-A	140	HIS
1	12-A	84	SER
1	12-A	140	HIS
1	13-A	14	ASP
1	13-A	17	ARG
1	13-A	36	VAL
1	13-A	43	ASN
1	13-A	69	LYS

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Mol	Chain	Res	Type
1	13-A	73	MSE
1	13-A	101	ASN
1	13-A	106	LEU
1	13-A	133	ILE
1	13-A	140	HIS
1	13-A	150	PRO
1	13-A	171	THR
1	13-A	175	ASN
1	14-A	6	LEU
1	14-A	10	ARG
1	14-A	67	ASN
1	14-A	96	LYS
1	14-A	140	HIS
1	14-A	141	ARG
1	14-A	150	PRO
1	14-A	164	CYS
1	14-A	170	ARG
1	15-A	14	ASP
1	15-A	28	VAL
1	15-A	61	ASN
1	15-A	69	LYS
1	15-A	70	PHE
1	15-A	73	MSE
1	15-A	96	LYS
1	15-A	120	LYS
1	15-A	140	HIS
1	15-A	150	PRO
1	16-A	14	ASP
1	16-A	69	LYS
1	16-A	73	MSE
1	16-A	110	PRO
1	16-A	140	HIS
1	16-A	141	ARG
1	16-A	150	PRO
1	16-A	175	ASN
1	16-A	179	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	129	GLN
1	3-A	115	ASN

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Mol	Chain	Res	Type
1	4-A	65	GLN
1	4-A	99	GLN
1	4-A	182	HIS
1	5-A	20	HIS
1	5-A	99	GLN
1	6-A	129	GLN
1	7-A	43	ASN
1	7-A	61	ASN
1	7-A	182	HIS
1	8-A	99	GLN
1	10-A	20	HIS
1	10-A	71	ASN
1	10-A	115	ASN
1	11-A	99	GLN
1	12-A	115	ASN
1	12-A	165	HIS
1	12-A	182	HIS
1	13-A	43	ASN
1	13-A	67	ASN
1	13-A	129	GLN
1	13-A	165	HIS
1	14-A	34	GLN
1	14-A	67	ASN
1	15-A	115	ASN
1	15-A	173	HIS
1	15-A	182	HIS
1	16-A	61	ASN
1	16-A	115	ASN
1	16-A	182	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	EDO	1-A	234	-	3,3,3	0.34	0	2,2,2	0.48	0
3	EDO	10-A	234	-	3,3,3	0.33	0	2,2,2	0.48	0
3	EDO	11-A	234	-	3,3,3	0.33	0	2,2,2	0.48	0
3	EDO	12-A	234	-	3,3,3	0.34	0	2,2,2	0.47	0
3	EDO	13-A	234	-	3,3,3	0.28	0	2,2,2	0.48	0
3	EDO	14-A	234	-	3,3,3	0.33	0	2,2,2	0.59	0
3	EDO	15-A	234	-	3,3,3	0.34	0	2,2,2	0.60	0
3	EDO	16-A	234	-	3,3,3	0.29	0	2,2,2	0.55	0
3	EDO	2-A	234	-	3,3,3	0.33	0	2,2,2	0.48	0
3	EDO	3-A	234	-	3,3,3	0.34	0	2,2,2	0.49	0
3	EDO	4-A	234	-	3,3,3	0.35	0	2,2,2	0.49	0
3	EDO	5-A	234	-	3,3,3	0.42	0	2,2,2	0.52	0
3	EDO	6-A	234	-	3,3,3	0.37	0	2,2,2	0.52	0
3	EDO	7-A	234	-	3,3,3	0.34	0	2,2,2	0.48	0
3	EDO	8-A	234	-	3,3,3	0.36	0	2,2,2	0.49	0
3	EDO	9-A	234	-	3,3,3	0.35	0	2,2,2	0.51	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	EDO	1-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	234	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	3-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	234	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	234	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	1-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	2-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	3-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	4-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	5-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	6-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	7-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	8-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	9-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	10-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	11-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	12-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	13-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	14-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	15-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
1	16-A	183/200 (91%)	-0.07	7 (3%)	44	50	5, 13, 29, 46	183 (100%)
All	All	2928/3200 (91%)	-0.07	112 (3%)	35	50	5, 13, 29, 46	2928 (100%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	118	ILE	7.7
1	2-A	118	ILE	7.7
1	3-A	118	ILE	7.7
1	4-A	118	ILE	7.7
1	5-A	118	ILE	7.7

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Mol	Chain	Res	Type	RSRZ
1	6-A	118	ILE	7.7
1	7-A	118	ILE	7.7
1	8-A	118	ILE	7.7
1	9-A	118	ILE	7.7
1	10-A	118	ILE	7.7
1	11-A	118	ILE	7.7
1	12-A	118	ILE	7.7
1	13-A	118	ILE	7.7
1	14-A	118	ILE	7.7
1	15-A	118	ILE	7.7
1	16-A	118	ILE	7.7
1	1-A	112	LYS	5.3
1	2-A	112	LYS	5.3
1	3-A	112	LYS	5.3
1	4-A	112	LYS	5.3
1	5-A	112	LYS	5.3
1	6-A	112	LYS	5.3
1	7-A	112	LYS	5.3
1	8-A	112	LYS	5.3
1	9-A	112	LYS	5.3
1	10-A	112	LYS	5.3
1	11-A	112	LYS	5.3
1	12-A	112	LYS	5.3
1	13-A	112	LYS	5.3
1	14-A	112	LYS	5.3
1	15-A	112	LYS	5.3
1	16-A	112	LYS	5.3
1	1-A	113	LYS	3.3
1	2-A	113	LYS	3.3
1	3-A	113	LYS	3.3
1	4-A	113	LYS	3.3
1	5-A	113	LYS	3.3
1	6-A	113	LYS	3.3
1	7-A	113	LYS	3.3
1	8-A	113	LYS	3.3
1	9-A	113	LYS	3.3
1	10-A	113	LYS	3.3
1	11-A	113	LYS	3.3
1	12-A	113	LYS	3.3
1	13-A	113	LYS	3.3
1	14-A	113	LYS	3.3
1	15-A	113	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	16-A	113	LYS	3.3
1	1-A	173	HIS	3.2
1	2-A	173	HIS	3.2
1	3-A	173	HIS	3.2
1	4-A	173	HIS	3.2
1	5-A	173	HIS	3.2
1	6-A	173	HIS	3.2
1	7-A	173	HIS	3.2
1	8-A	173	HIS	3.2
1	9-A	173	HIS	3.2
1	10-A	173	HIS	3.2
1	11-A	173	HIS	3.2
1	12-A	173	HIS	3.2
1	13-A	173	HIS	3.2
1	14-A	173	HIS	3.2
1	15-A	173	HIS	3.2
1	16-A	173	HIS	3.2
1	1-A	111	ASP	2.5
1	2-A	111	ASP	2.5
1	3-A	111	ASP	2.5
1	4-A	111	ASP	2.5
1	5-A	111	ASP	2.5
1	6-A	111	ASP	2.5
1	7-A	111	ASP	2.5
1	8-A	111	ASP	2.5
1	9-A	111	ASP	2.5
1	10-A	111	ASP	2.5
1	11-A	111	ASP	2.5
1	12-A	111	ASP	2.5
1	13-A	111	ASP	2.5
1	14-A	111	ASP	2.5
1	15-A	111	ASP	2.5
1	16-A	111	ASP	2.5
1	1-A	115	ASN	2.5
1	2-A	115	ASN	2.5
1	3-A	115	ASN	2.5
1	4-A	115	ASN	2.5
1	5-A	115	ASN	2.5
1	6-A	115	ASN	2.5
1	7-A	115	ASN	2.5
1	8-A	115	ASN	2.5
1	9-A	115	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	10-A	115	ASN	2.5
1	11-A	115	ASN	2.5
1	12-A	115	ASN	2.5
1	13-A	115	ASN	2.5
1	14-A	115	ASN	2.5
1	15-A	115	ASN	2.5
1	16-A	115	ASN	2.5
1	1-A	171	THR	2.3
1	2-A	171	THR	2.3
1	3-A	171	THR	2.3
1	4-A	171	THR	2.3
1	5-A	171	THR	2.3
1	6-A	171	THR	2.3
1	7-A	171	THR	2.3
1	8-A	171	THR	2.3
1	9-A	171	THR	2.3
1	10-A	171	THR	2.3
1	11-A	171	THR	2.3
1	12-A	171	THR	2.3
1	13-A	171	THR	2.3
1	14-A	171	THR	2.3
1	15-A	171	THR	2.3
1	16-A	171	THR	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NI	14-A	201	1/1	1.00	0.03	-4.05	16,16,16,16	1
2	NI	16-A	201	1/1	1.00	0.03	-4.05	16,16,16,16	1
2	NI	1-A	201	1/1	1.00	0.03	-4.14	14,14,14,14	1
2	NI	15-A	201	1/1	1.00	0.03	-4.18	0,0,0,0	1
2	NI	8-A	201	1/1	1.00	0.03	-4.34	11,11,11,11	1
2	NI	3-A	201	1/1	1.00	0.03	-4.34	8,8,8,8	1
2	NI	2-A	201	1/1	1.00	0.03	-4.34	12,12,12,12	1
2	NI	7-A	201	1/1	1.00	0.03	-4.34	12,12,12,12	1
2	NI	6-A	201	1/1	1.00	0.03	-4.34	13,13,13,13	1
2	NI	4-A	201	1/1	1.00	0.03	-4.34	14,14,14,14	1
2	NI	9-A	201	1/1	1.00	0.03	-4.34	8,8,8,8	1
2	NI	5-A	201	1/1	1.00	0.03	-4.55	15,15,15,15	1
2	NI	12-A	201	1/1	1.00	0.03	-4.55	0,0,0,0	1
2	NI	13-A	201	1/1	1.00	0.03	-4.55	15,15,15,15	1
2	NI	11-A	201	1/1	1.00	0.03	-4.64	15,15,15,15	1
3	EDO	16-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	6-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	4-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	2-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	12-A	234	4/4	0.90	0.15	-	35,37,39,39	4
3	EDO	15-A	234	4/4	0.90	0.15	-	35,37,39,40	4
2	NI	10-A	201	1/1	1.00	0.03	-	14,14,14,14	1
3	EDO	13-A	234	4/4	0.90	0.15	-	35,37,39,39	4
3	EDO	11-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	14-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	10-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	3-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	1-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	8-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	9-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	7-A	234	4/4	0.90	0.15	-	35,37,39,40	4
3	EDO	5-A	234	4/4	0.90	0.15	-	35,37,39,40	4

6.5 Other polymers

There are no such residues in this entry.