



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:17 PM UTC

PDB ID : 4YRR / pdb_00004yrr
Title : Crystal structure of T. cruzi Histidyl-tRNA synthetase in complex with N-(quinolin-3-yl)acetamide (Chem 1691)
Authors : Koh, C.-Y.; Hol, W.G.J.
Deposited on : 2015-03-15
Resolution : 2.30 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

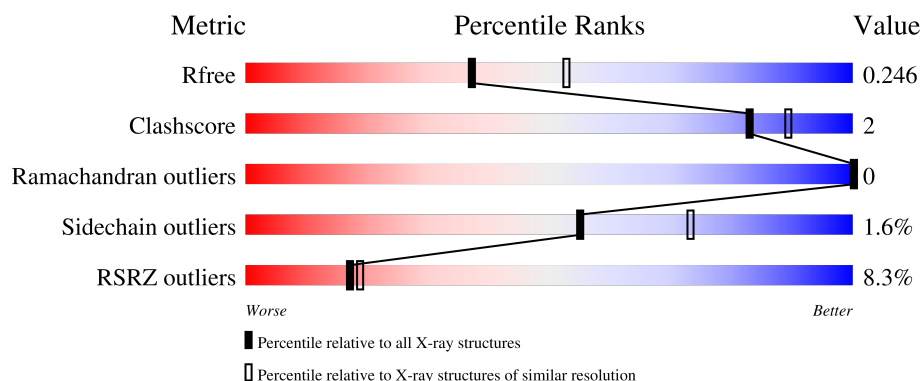
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	456	7% 85% 5% 10%
1	B	456	8% 84% 5% 11%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6621 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 Histidyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	2	0
			3159	2021	544	578	16			
1	B	406	Total	C	N	O	S	0	1	0
			3110	1988	535	570	17			

There are 44 discrepancies between the modelled and reference sequences:

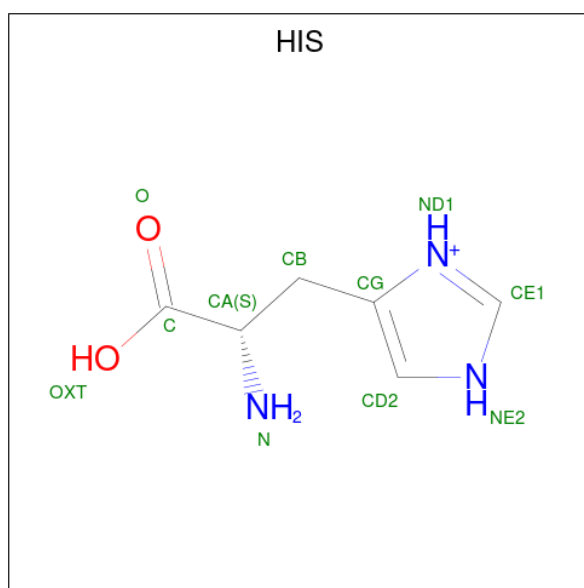
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q4DA54
A	-20	ALA	-	expression tag	UNP Q4DA54
A	-19	HIS	-	expression tag	UNP Q4DA54
A	-18	HIS	-	expression tag	UNP Q4DA54
A	-17	HIS	-	expression tag	UNP Q4DA54
A	-16	HIS	-	expression tag	UNP Q4DA54
A	-15	HIS	-	expression tag	UNP Q4DA54
A	-14	HIS	-	expression tag	UNP Q4DA54
A	-13	MET	-	expression tag	UNP Q4DA54
A	-12	GLY	-	expression tag	UNP Q4DA54
A	-11	THR	-	expression tag	UNP Q4DA54
A	-10	LEU	-	expression tag	UNP Q4DA54
A	-9	GLU	-	expression tag	UNP Q4DA54
A	-8	ALA	-	expression tag	UNP Q4DA54
A	-7	GLN	-	expression tag	UNP Q4DA54
A	-6	THR	-	expression tag	UNP Q4DA54
A	-5	GLN	-	expression tag	UNP Q4DA54
A	-4	GLY	-	expression tag	UNP Q4DA54
A	-3	PRO	-	expression tag	UNP Q4DA54
A	-2	GLY	-	expression tag	UNP Q4DA54
A	-1	SER	-	expression tag	UNP Q4DA54
A	0	MET	-	expression tag	UNP Q4DA54
B	-21	MET	-	initiating methionine	UNP Q4DA54
B	-20	ALA	-	expression tag	UNP Q4DA54
B	-19	HIS	-	expression tag	UNP Q4DA54

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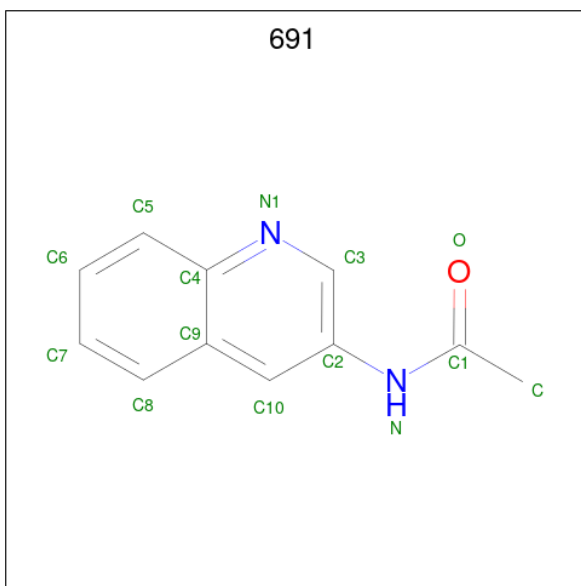
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP Q4DA54
B	-17	HIS	-	expression tag	UNP Q4DA54
B	-16	HIS	-	expression tag	UNP Q4DA54
B	-15	HIS	-	expression tag	UNP Q4DA54
B	-14	HIS	-	expression tag	UNP Q4DA54
B	-13	MET	-	expression tag	UNP Q4DA54
B	-12	GLY	-	expression tag	UNP Q4DA54
B	-11	THR	-	expression tag	UNP Q4DA54
B	-10	LEU	-	expression tag	UNP Q4DA54
B	-9	GLU	-	expression tag	UNP Q4DA54
B	-8	ALA	-	expression tag	UNP Q4DA54
B	-7	GLN	-	expression tag	UNP Q4DA54
B	-6	THR	-	expression tag	UNP Q4DA54
B	-5	GLN	-	expression tag	UNP Q4DA54
B	-4	GLY	-	expression tag	UNP Q4DA54
B	-3	PRO	-	expression tag	UNP Q4DA54
B	-2	GLY	-	expression tag	UNP Q4DA54
B	-1	SER	-	expression tag	UNP Q4DA54
B	0	MET	-	expression tag	UNP Q4DA54

- Molecule 2 is HISTIDINE (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



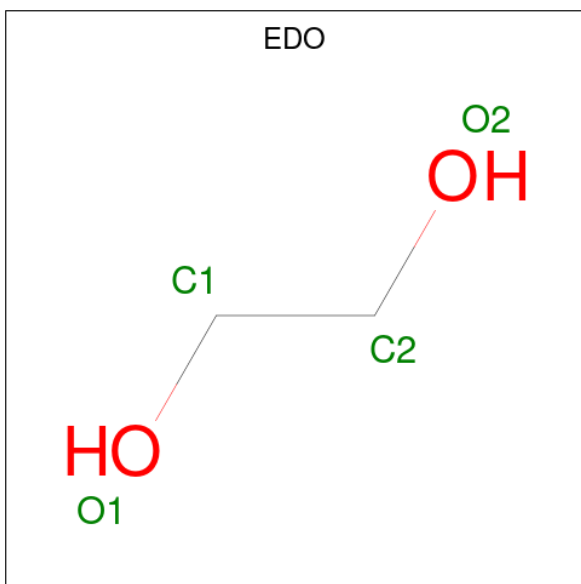
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	3	2		
2	B	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 3 is N-(quinolin-3-yl)acetamide (CCD ID: 691) (formula: $C_{11}H_{10}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			28	22	4	2		
3	B	1	Total	C	N	O	0	1
			28	22	4	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



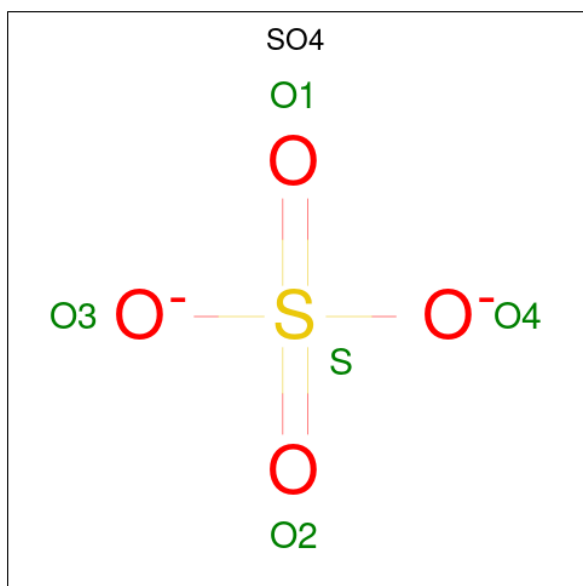
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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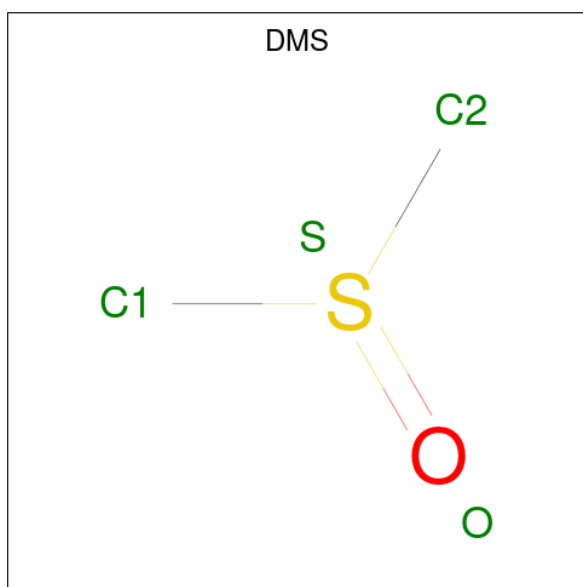
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

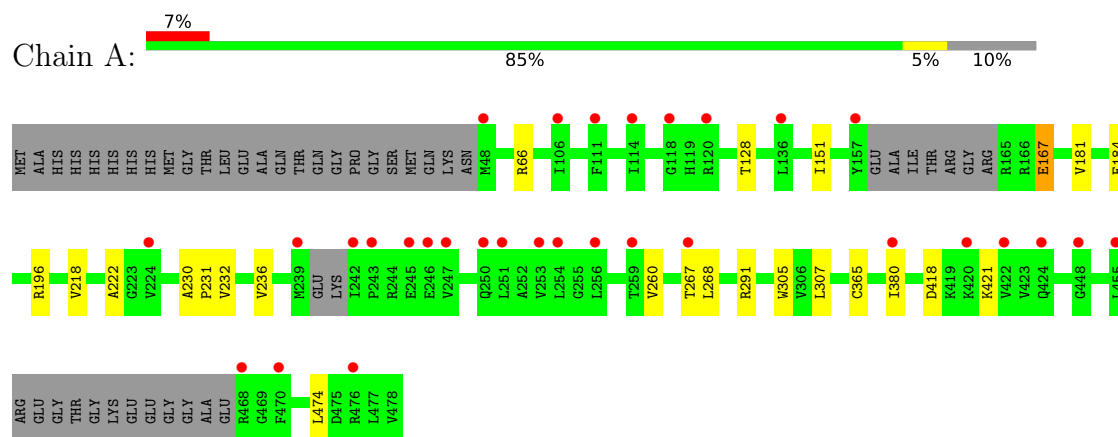
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	109	Total	O	0	0
			109	109		
7	B	116	Total	O	0	0
			116	116		

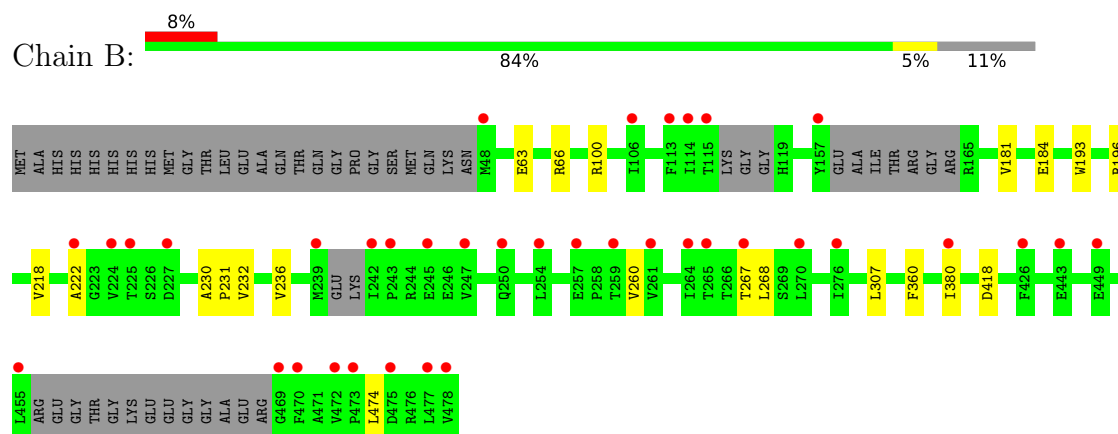
3 Residue-property plots [i](#)

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: Histidyl-tRNA synthetase



- Molecule 1: Histidyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.01Å 118.43Å 93.81Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	36.15 – 2.30 36.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.15-2.30) 99.7 (36.15-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.29Å)	Xtriage
Refinement program	REFMAC refmac _5.8.0073	Depositor
R, R_{free}	0.217 , 0.245 0.220 , 0.246	Depositor DCC
R_{free} test set	2229 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6621	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.75 % 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 1.4413e-06. 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: 691, EDO, DMS, SO4

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	0.53	1/3231 (0.0%)	0.74	1/4384 (0.0%)
1	B	0.52	0/3176	0.74	0/4311
All	All	0.53	1/6407 (0.0%)	0.74	1/8695 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	CA-C	5.02	1.58	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	GLU	N-CA-CB	-5.02	102.38	110.71

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	3159	0	3092	12	0
1	B	3110	0	3029	14	0
2	A	11	0	6	1	0
2	B	11	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	20	4	0
3	B	28	0	20	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	15	0	0	1	0
5	B	10	0	0	0	0
6	A	8	0	12	0	0
6	B	8	0	12	4	0
7	A	109	0	0	0	1
7	B	116	0	0	0	1
All	All	6621	0	6209	30	1

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 2.

All (30) 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:66:ARG:NE	1:A:380:ILE:O	2.29	0.65
1:B:66:ARG:NE	1:B:380:ILE:O	2.28	0.65
1:A:230:ALA:HB3	1:A:231:PRO:HD3	1.82	0.62
1:B:230:ALA:HB3	1:B:231:PRO:HD3	1.82	0.61
3:A:502[B]:691:H6	3:A:502[B]:691:O	2.03	0.59
1:A:196:ARG:HD2	1:A:305:TRP:HZ2	1.70	0.57
3:B:502[B]:691:H6	3:B:502[B]:691:O	2.04	0.56
1:B:100:ARG:HG2	6:B:507:DMS:H13	1.86	0.56
1:A:218:VAL:HG21	1:A:267:THR:HG21	1.90	0.54
1:B:218:VAL:HG21	1:B:267:THR:HG21	1.91	0.53
1:A:128:THR:HG1	2:A:501:HIS:N	2.08	0.52
1:B:196:ARG:HG2	6:B:506:DMS:C1	2.41	0.51
1:A:236:VAL:CG1	1:A:268:LEU:HD11	2.41	0.50
1:B:236:VAL:CG1	1:B:268:LEU:HD11	2.41	0.50
1:A:232:VAL:O	1:A:236:VAL:HG23	2.11	0.49
1:B:232:VAL:O	1:B:236:VAL:HG23	2.12	0.49
3:A:502[B]:691:H1	5:A:505:SO4:O3	2.13	0.48
1:B:222:ALA:HB1	1:B:260:VAL:HG22	1.96	0.47
1:A:236:VAL:HG13	1:A:268:LEU:HD11	1.97	0.47
1:B:193:TRP:CE2	6:B:506:DMS:H22	2.51	0.46
1:A:222:ALA:HB1	1:A:260:VAL:HG22	1.96	0.46
1:A:365:CYS:CB	3:A:502[A]:691:H3	2.46	0.45
3:A:502[A]:691:H5	3:A:502[A]:691:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:VAL:HA	1:B:184:GLU:OE2	2.17	0.44
1:B:236:VAL:HG13	1:B:268:LEU:HD11	1.99	0.44
1:A:181:VAL:HA	1:A:184:GLU:OE2	2.18	0.42
1:A:230:ALA:HB3	1:A:231:PRO:CD	2.48	0.42
1:B:360:PHE:CD1	1:B:360:PHE:C	2.97	0.42
1:B:196:ARG:HH11	6:B:506:DMS:H11	1.85	0.42
1:B:230:ALA:HB3	1:B:231:PRO:CD	2.48	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:637:HOH:O	7:B:708:HOH:O[4_546]	2.03	0.17

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	404/456 (89%)	395 (98%)	9 (2%)	0	100	100
1	B	397/456 (87%)	389 (98%)	8 (2%)	0	100	100
All	All	801/912 (88%)	784 (98%)	17 (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	325/380 (86%)	319 (98%)	6 (2%)	51	70
1	B	318/380 (84%)	314 (99%)	4 (1%)	61	77
All	All	643/760 (85%)	633 (98%)	10 (2%)	55	73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	GLU
1	A	291	ARG
1	A	307	LEU
1	A	418	ASP
1	A	421	LYS
1	A	474	LEU
1	B	63	GLU
1	B	307	LEU
1	B	418	ASP
1	B	474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	B	216	GLN
1	B	296	GLN
1	B	424	GLN
1	B	427	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

17 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
5	SO4	A	506	-	4,4,4	0.43	0	6,6,6	0.23	0
5	SO4	A	505	-	4,4,4	0.44	0	6,6,6	0.31	0
4	EDO	A	503	-	3,3,3	0.35	0	2,2,2	0.72	0
3	691	B	502[A]	-	15,15,15	0.17	0	20,20,20	1.01	2 (10%)
6	DMS	B	506	-	3,3,3	0.68	0	3,3,3	0.48	0
4	EDO	B	503	-	3,3,3	0.44	0	2,2,2	0.31	0
3	691	A	502[A]	-	15,15,15	0.18	0	20,20,20	0.96	2 (10%)
5	SO4	B	505	-	4,4,4	0.46	0	6,6,6	0.47	0
5	SO4	B	504	-	4,4,4	0.41	0	6,6,6	0.29	0
2	HIS	B	501	-	10,11,11	0.75	1 (10%)	10,14,14	1.10	0
6	DMS	A	507	-	3,3,3	0.58	0	3,3,3	0.59	0
6	DMS	B	507	-	3,3,3	0.56	0	3,3,3	0.62	0
5	SO4	A	504	-	4,4,4	0.52	0	6,6,6	0.68	0
3	691	B	502[B]	-	15,15,15	0.16	0	20,20,20	0.99	2 (10%)
6	DMS	A	508	-	3,3,3	0.57	0	3,3,3	0.53	0
2	HIS	A	501	-	10,11,11	0.82	1 (10%)	10,14,14	1.22	1 (10%)
3	691	A	502[B]	-	15,15,15	0.17	0	20,20,20	1.02	2 (10%)

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	EDO	A	503	-	-	0/1/1/1	-
3	691	B	502[A]	-	-	2/4/4/4	0/2/2/2
4	EDO	B	503	-	-	1/1/1/1	-
3	691	A	502[A]	-	-	0/4/4/4	0/2/2/2
2	HIS	B	501	-	-	0/8/8/8	0/1/1/1
3	691	B	502[B]	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIS	A	501	-	-	0/8/8/8	0/1/1/1
3	691	A	502[B]	-	-	0/4/4/4	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HIS	OXT-C	-2.35	1.23	1.30
2	B	501	HIS	OXT-C	-2.03	1.24	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[A]	691	C2-C3-N1	3.50	127.19	124.52
3	A	502[B]	691	C2-C3-N1	3.49	127.19	124.52
3	B	502[B]	691	C2-C3-N1	3.41	127.12	124.52
3	A	502[A]	691	C2-C3-N1	3.24	127.00	124.52
3	A	502[B]	691	C10-C2-C3	-2.74	116.14	118.18
3	B	502[A]	691	C10-C2-C3	-2.66	116.20	118.18
3	B	502[B]	691	C10-C2-C3	-2.61	116.23	118.18
3	A	502[A]	691	C10-C2-C3	-2.59	116.25	118.18
2	A	501	HIS	OXT-C-O	-2.45	118.51	124.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502[A]	691	O-C1-N-C2
3	B	502[A]	691	C-C1-N-C2
4	B	503	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	SO4	1	0
6	B	506	DMS	3	0
3	A	502[A]	691	2	0
6	B	507	DMS	1	0
3	B	502[B]	691	1	0
2	A	501	HIS	1	0
3	A	502[B]	691	2	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 ⓘ

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	410/456 (89%)	0.51	31 (7%)	20 21	13, 42, 84, 111	2 (0%)
1	B	406/456 (89%)	0.51	37 (9%)	15 16	14, 41, 85, 117	1 (0%)
All	All	816/912 (89%)	0.51	68 (8%)	17 19	13, 41, 85, 117	3 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	MET	4.8
1	B	157	TYR	4.6
1	A	239	MET	4.2
1	A	247	VAL	4.2
1	A	470	PHE	4.0
1	A	254	LEU	3.7
1	B	225	THR	3.5
1	B	254	LEU	3.4
1	B	276	ILE	3.3
1	A	259	THR	3.3
1	B	478	VAL	3.3
1	B	261	VAL	3.3
1	A	118	GLY	3.2
1	B	242	ILE	3.2
1	A	380	ILE	3.2
1	B	113	PHE	3.2
1	B	475	ASP	3.1
1	B	247	VAL	3.1
1	B	455	LEU	3.1
1	A	253	VAL	3.0
1	A	256	LEU	2.9
1	A	242	ILE	2.9
1	A	157	TYR	2.9
1	B	48	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	227	ASP	2.8
1	A	114	ILE	2.7
1	B	267	THR	2.7
1	A	455	LEU	2.7
1	B	250	GLN	2.7
1	B	115	THR	2.7
1	B	243	PRO	2.7
1	B	114	ILE	2.6
1	A	224	VAL	2.5
1	A	106	ILE	2.5
1	A	424	GLN	2.5
1	A	251	LEU	2.5
1	A	468	ARG	2.5
1	A	243	PRO	2.5
1	A	250	GLN	2.4
1	A	267	THR	2.4
1	A	120	ARG	2.4
1	A	448	GLY	2.4
1	B	380	ILE	2.4
1	B	426	PHE	2.4
1	A	136	LEU	2.4
1	B	449	GLU	2.4
1	B	270	LEU	2.3
1	B	257	GLU	2.3
1	B	469	GLY	2.3
1	B	259	THR	2.3
1	A	246	GLU	2.3
1	A	111	PHE	2.2
1	B	470	PHE	2.2
1	A	48	MET	2.2
1	B	443	GLU	2.2
1	A	420	LYS	2.2
1	B	222	ALA	2.2
1	A	476	ARG	2.1
1	B	106	ILE	2.1
1	B	264	ILE	2.1
1	B	245	GLU	2.1
1	A	422	VAL	2.1
1	B	224	VAL	2.1
1	B	472	VAL	2.1
1	B	265	THR	2.1
1	B	473	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	245	GLU	2.0
1	B	477	LEU	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	EDO	A	503	4/4	0.77	0.19	50,52,53,54	0
4	EDO	B	503	4/4	0.78	0.20	47,49,51,52	0
3	691	B	502[A]	14/14	0.79	0.18	46,49,54,55	14
3	691	B	502[B]	14/14	0.79	0.18	52,53,59,60	14
3	691	A	502[A]	14/14	0.79	0.14	44,46,50,51	14
3	691	A	502[B]	14/14	0.79	0.14	53,55,62,63	14
6	DMS	B	506	4/4	0.84	0.19	53,54,59,60	0
5	SO4	A	504	5/5	0.86	0.13	42,43,50,51	0
6	DMS	B	507	4/4	0.86	0.20	72,72,73,75	0
6	DMS	A	508	4/4	0.87	0.16	70,71,72,73	0
5	SO4	A	505	5/5	0.87	0.24	66,71,74,75	0
5	SO4	B	505	5/5	0.87	0.12	46,48,49,50	0
6	DMS	A	507	4/4	0.89	0.16	54,56,58,58	0
5	SO4	A	506	5/5	0.90	0.10	47,49,52,53	0
5	SO4	B	504	5/5	0.91	0.17	57,57,59,61	0
2	HIS	B	501	11/11	0.94	0.08	23,24,27,29	0
2	HIS	A	501	11/11	0.94	0.08	22,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.