



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:49 PM UTC

PDB ID : 4JX4 / pdb_00004jx4
Title : Structure of the carboxyl transferase domain from *Rhizobium etli* pyruvate carboxylase
Authors : Lietzan, A.D.; St Maurice, M.
Deposited on : 2013-03-27
Resolution : 2.98 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

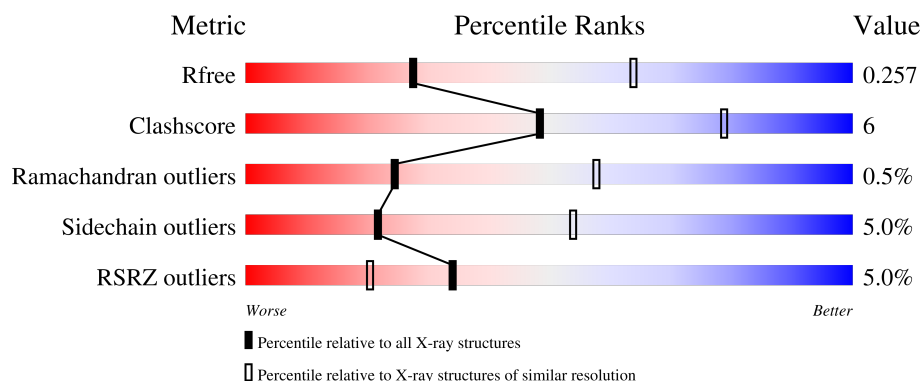
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	632	 79% 14% • 6%
1	B	632	 81% 12% • 6%
1	C	632	 80% 12% • 6%
1	D	632	 83% 10% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17166 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	1	0
			4450	2831	740	856	23			
1	B	595	Total	C	N	O	S	0	0	0
			4268	2699	716	831	22			
1	C	595	Total	C	N	O	S	0	0	0
			4325	2730	730	843	22			
1	D	594	Total	C	N	O	S	0	0	0
			4117	2573	704	818	22			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	expression tag	UNP Q2K340
A	437	GLY	-	expression tag	UNP Q2K340
A	438	SER	-	expression tag	UNP Q2K340
A	439	SER	-	expression tag	UNP Q2K340
A	440	HIS	-	expression tag	UNP Q2K340
A	441	HIS	-	expression tag	UNP Q2K340
A	442	HIS	-	expression tag	UNP Q2K340
A	443	HIS	-	expression tag	UNP Q2K340
A	444	HIS	-	expression tag	UNP Q2K340
A	445	HIS	-	expression tag	UNP Q2K340
A	446	HIS	-	expression tag	UNP Q2K340
A	447	HIS	-	expression tag	UNP Q2K340
A	448	ASP	-	expression tag	UNP Q2K340
A	449	TYR	-	expression tag	UNP Q2K340
A	450	ASP	-	expression tag	UNP Q2K340
A	451	ILE	-	expression tag	UNP Q2K340
A	452	PRO	-	expression tag	UNP Q2K340
A	453	THR	-	expression tag	UNP Q2K340
A	454	SER	-	expression tag	UNP Q2K340
A	455	GLU	-	expression tag	UNP Q2K340
A	456	ASN	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	expression tag	UNP Q2K340
A	458	TYR	-	expression tag	UNP Q2K340
A	459	PHE	-	expression tag	UNP Q2K340
A	460	GLN	-	expression tag	UNP Q2K340
A	461	GLY	-	expression tag	UNP Q2K340
A	462	LEU	-	expression tag	UNP Q2K340
A	463	LEU	-	expression tag	UNP Q2K340
A	464	HIS	-	expression tag	UNP Q2K340
B	436	MET	-	expression tag	UNP Q2K340
B	437	GLY	-	expression tag	UNP Q2K340
B	438	SER	-	expression tag	UNP Q2K340
B	439	SER	-	expression tag	UNP Q2K340
B	440	HIS	-	expression tag	UNP Q2K340
B	441	HIS	-	expression tag	UNP Q2K340
B	442	HIS	-	expression tag	UNP Q2K340
B	443	HIS	-	expression tag	UNP Q2K340
B	444	HIS	-	expression tag	UNP Q2K340
B	445	HIS	-	expression tag	UNP Q2K340
B	446	HIS	-	expression tag	UNP Q2K340
B	447	HIS	-	expression tag	UNP Q2K340
B	448	ASP	-	expression tag	UNP Q2K340
B	449	TYR	-	expression tag	UNP Q2K340
B	450	ASP	-	expression tag	UNP Q2K340
B	451	ILE	-	expression tag	UNP Q2K340
B	452	PRO	-	expression tag	UNP Q2K340
B	453	THR	-	expression tag	UNP Q2K340
B	454	SER	-	expression tag	UNP Q2K340
B	455	GLU	-	expression tag	UNP Q2K340
B	456	ASN	-	expression tag	UNP Q2K340
B	457	LEU	-	expression tag	UNP Q2K340
B	458	TYR	-	expression tag	UNP Q2K340
B	459	PHE	-	expression tag	UNP Q2K340
B	460	GLN	-	expression tag	UNP Q2K340
B	461	GLY	-	expression tag	UNP Q2K340
B	462	LEU	-	expression tag	UNP Q2K340
B	463	LEU	-	expression tag	UNP Q2K340
B	464	HIS	-	expression tag	UNP Q2K340
C	436	MET	-	expression tag	UNP Q2K340
C	437	GLY	-	expression tag	UNP Q2K340
C	438	SER	-	expression tag	UNP Q2K340
C	439	SER	-	expression tag	UNP Q2K340
C	440	HIS	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	441	HIS	-	expression tag	UNP Q2K340
C	442	HIS	-	expression tag	UNP Q2K340
C	443	HIS	-	expression tag	UNP Q2K340
C	444	HIS	-	expression tag	UNP Q2K340
C	445	HIS	-	expression tag	UNP Q2K340
C	446	HIS	-	expression tag	UNP Q2K340
C	447	HIS	-	expression tag	UNP Q2K340
C	448	ASP	-	expression tag	UNP Q2K340
C	449	TYR	-	expression tag	UNP Q2K340
C	450	ASP	-	expression tag	UNP Q2K340
C	451	ILE	-	expression tag	UNP Q2K340
C	452	PRO	-	expression tag	UNP Q2K340
C	453	THR	-	expression tag	UNP Q2K340
C	454	SER	-	expression tag	UNP Q2K340
C	455	GLU	-	expression tag	UNP Q2K340
C	456	ASN	-	expression tag	UNP Q2K340
C	457	LEU	-	expression tag	UNP Q2K340
C	458	TYR	-	expression tag	UNP Q2K340
C	459	PHE	-	expression tag	UNP Q2K340
C	460	GLN	-	expression tag	UNP Q2K340
C	461	GLY	-	expression tag	UNP Q2K340
C	462	LEU	-	expression tag	UNP Q2K340
C	463	LEU	-	expression tag	UNP Q2K340
C	464	HIS	-	expression tag	UNP Q2K340
D	436	MET	-	expression tag	UNP Q2K340
D	437	GLY	-	expression tag	UNP Q2K340
D	438	SER	-	expression tag	UNP Q2K340
D	439	SER	-	expression tag	UNP Q2K340
D	440	HIS	-	expression tag	UNP Q2K340
D	441	HIS	-	expression tag	UNP Q2K340
D	442	HIS	-	expression tag	UNP Q2K340
D	443	HIS	-	expression tag	UNP Q2K340
D	444	HIS	-	expression tag	UNP Q2K340
D	445	HIS	-	expression tag	UNP Q2K340
D	446	HIS	-	expression tag	UNP Q2K340
D	447	HIS	-	expression tag	UNP Q2K340
D	448	ASP	-	expression tag	UNP Q2K340
D	449	TYR	-	expression tag	UNP Q2K340
D	450	ASP	-	expression tag	UNP Q2K340
D	451	ILE	-	expression tag	UNP Q2K340
D	452	PRO	-	expression tag	UNP Q2K340
D	453	THR	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	expression tag	UNP Q2K340
D	455	GLU	-	expression tag	UNP Q2K340
D	456	ASN	-	expression tag	UNP Q2K340
D	457	LEU	-	expression tag	UNP Q2K340
D	458	TYR	-	expression tag	UNP Q2K340
D	459	PHE	-	expression tag	UNP Q2K340
D	460	GLN	-	expression tag	UNP Q2K340
D	461	GLY	-	expression tag	UNP Q2K340
D	462	LEU	-	expression tag	UNP Q2K340
D	463	LEU	-	expression tag	UNP Q2K340
D	464	HIS	-	expression tag	UNP Q2K340

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

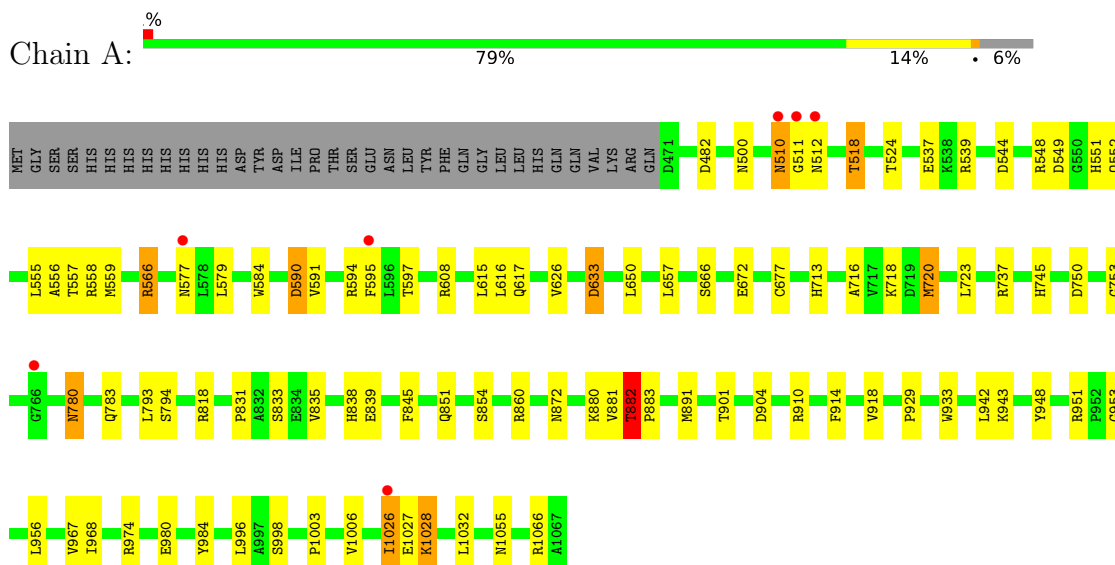
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0

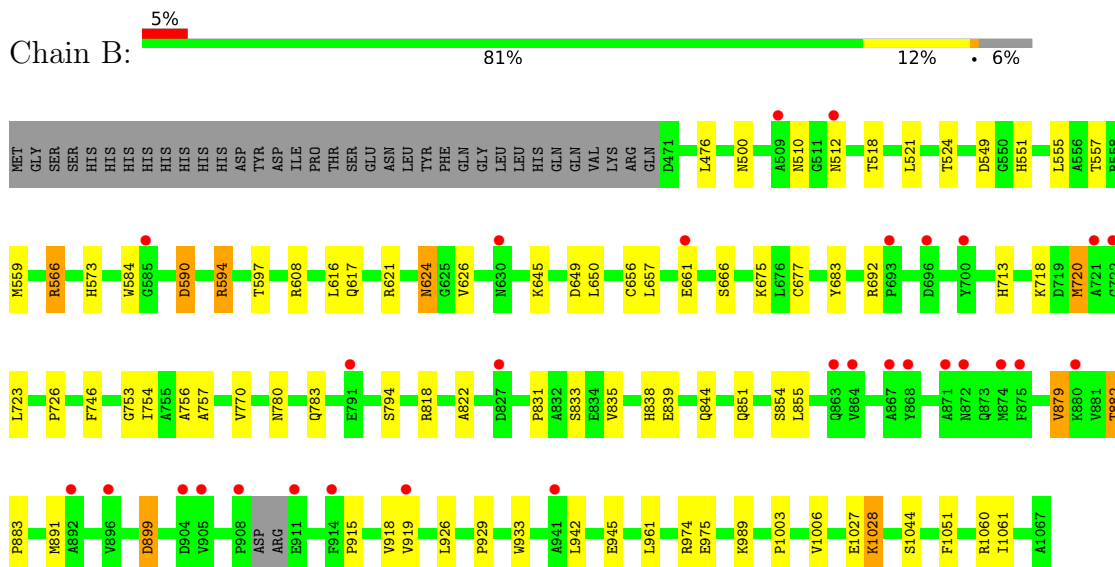
3 Residue-property plots [i](#)

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: Pyruvate carboxylase

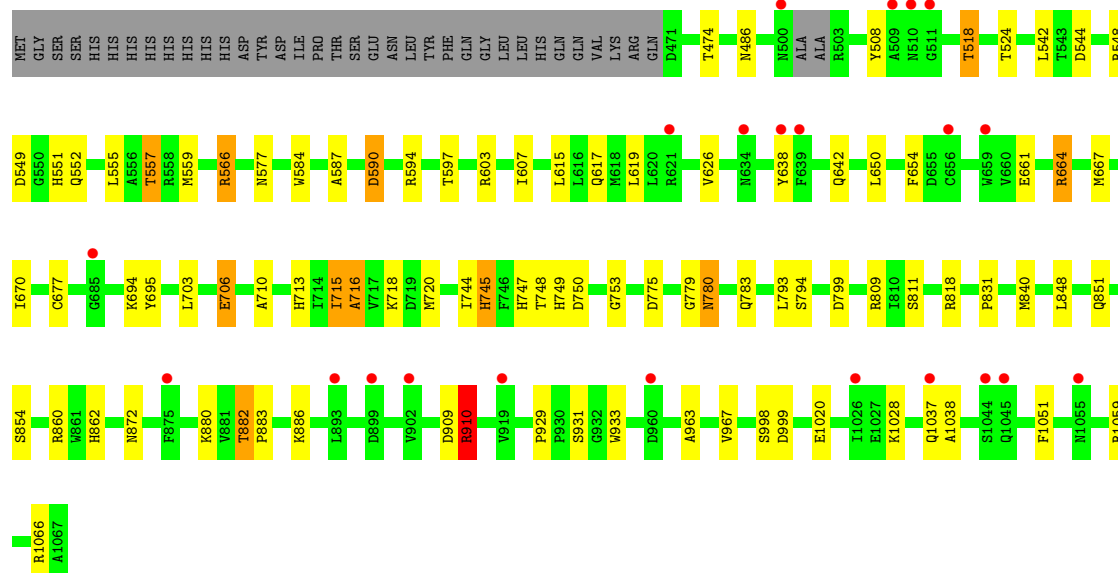


- Molecule 1: Pyruvate carboxylase



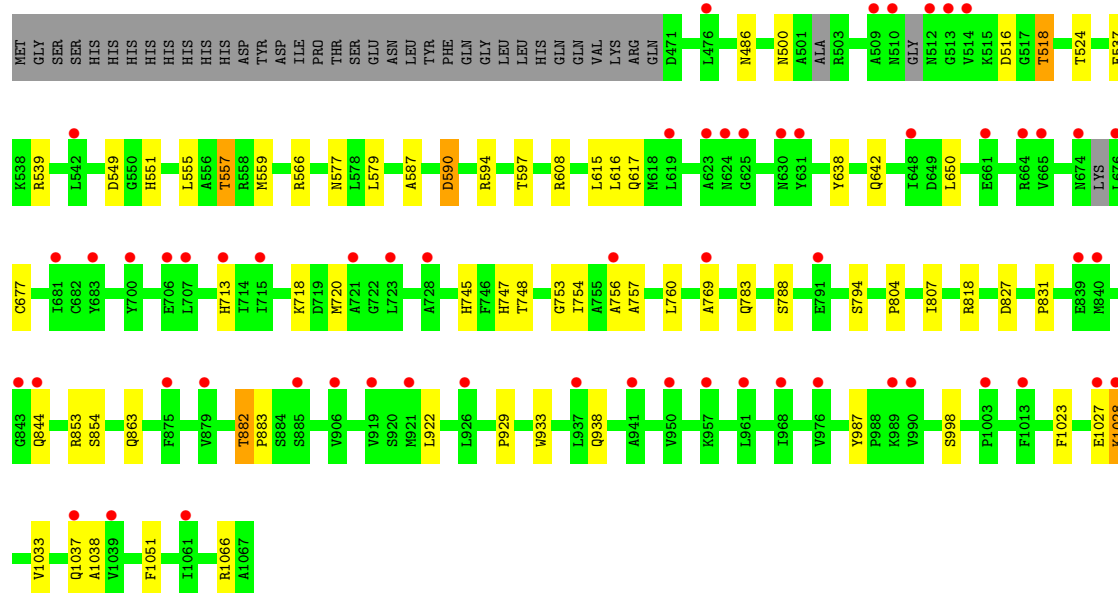
- Molecule 1: Pyruvate carboxylase

Chain C:  3% 80% 12% 6%



• Molecule 1: Pyruvate carboxylase

Chain D:  9% 83% 10% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.21Å 157.23Å 245.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.98 50.00 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.98) 99.8 (50.00-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.248 (Not available) , 0.257	Depositor DCC
R_{free} test set	3481 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17166	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: ZN, KCX, CL

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	0.95	0/4536	1.07	7/6189 (0.1%)
1	B	0.85	2/4349 (0.0%)	0.99	5/5957 (0.1%)
1	C	0.94	7/4409 (0.2%)	1.01	6/6026 (0.1%)
1	D	0.78	1/4193 (0.0%)	0.97	1/5743 (0.0%)
All	All	0.89	10/17487 (0.1%)	1.01	19/23915 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	749	HIS	CG-CD2	7.26	1.43	1.35
1	C	745	HIS	CG-CD2	6.46	1.43	1.35
1	C	715	ILE	CA-C	6.20	1.60	1.52
1	B	899	ASP	CG-OD1	6.12	1.36	1.25
1	C	747	HIS	CG-CD2	5.76	1.42	1.35
1	C	862	HIS	CG-CD2	5.76	1.42	1.35
1	C	910	ARG	NE-CZ	5.70	1.39	1.33
1	C	716	ALA	N-CA	-5.30	1.39	1.46
1	D	747	HIS	CG-CD2	5.19	1.41	1.35
1	B	573	HIS	CG-CD2	5.18	1.41	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	951	ARG	NE-CZ-NH2	10.37	128.53	119.20
1	A	951	ARG	NE-CZ-NH1	-8.38	113.12	121.50
1	B	594	ARG	NE-CZ-NH2	-7.16	112.76	119.20
1	A	951	ARG	CD-NE-CZ	7.13	134.39	124.40
1	A	626	VAL	N-CA-C	-6.96	106.52	113.20
1	C	626	VAL	N-CA-C	-6.46	107.00	113.20
1	B	594	ARG	NE-CZ-NH1	6.18	127.68	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	748	THR	N-CA-C	5.98	117.29	108.86
1	B	594	ARG	CD-NE-CZ	5.90	132.66	124.40
1	C	780	ASN	CB-CA-C	-5.53	110.19	116.54
1	A	626	VAL	CB-CA-C	-5.52	105.24	110.70
1	A	780	ASN	CB-CA-C	-5.51	110.24	116.63
1	A	882	THR	CB-CA-C	-5.30	101.39	109.50
1	B	780	ASN	CB-CA-C	-5.20	110.59	116.63
1	C	748	THR	N-CA-C	5.13	116.09	108.86
1	C	799	ASP	CA-C-N	5.06	124.67	119.56
1	C	799	ASP	C-N-CA	5.06	124.67	119.56
1	B	645	LYS	N-CA-C	-5.05	105.77	111.28
1	C	1020	GLU	N-CA-C	5.00	117.48	110.23

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	4450	0	4253	52	1
1	B	4268	0	3880	45	0
1	C	4325	0	3933	50	0
1	D	4117	0	3501	45	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	17166	0	15567	180	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 6.

All (180) 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:C:677:CYS:H	1:C:713:HIS:HD2	0.97	0.97
1:D:677:CYS:H	1:D:713:HIS:HD2	0.95	0.95
1:A:723:LEU:HD11	1:A:839:GLU:HG2	1.51	0.92
1:B:677:CYS:H	1:B:713:HIS:HD2	0.96	0.92
1:C:664:ARG:HH11	1:C:664:ARG:HG3	1.33	0.92
1:A:677:CYS:H	1:A:713:HIS:HD2	1.00	0.91
1:D:677:CYS:H	1:D:713:HIS:CD2	1.88	0.91
1:C:664:ARG:HH11	1:C:664:ARG:CG	1.83	0.90
1:B:677:CYS:H	1:B:713:HIS:CD2	1.89	0.89
1:C:677:CYS:H	1:C:713:HIS:CD2	1.90	0.84
1:A:677:CYS:H	1:A:713:HIS:CD2	1.92	0.83
1:D:590:ASP:OD1	1:D:594:ARG:NH2	2.17	0.78
1:A:590:ASP:OD1	1:A:594:ARG:NH2	2.18	0.77
1:B:677:CYS:N	1:B:713:HIS:HD2	1.81	0.74
1:A:723:LEU:CD1	1:A:839:GLU:HG2	2.17	0.74
1:B:656:CYS:O	1:B:879:VAL:HG13	1.88	0.73
1:C:664:ARG:HG3	1:C:664:ARG:NH1	2.02	0.73
1:B:915:PRO:HB2	1:B:918:VAL:HG23	1.71	0.73
1:C:590:ASP:OD1	1:C:594:ARG:NH2	2.21	0.72
1:C:1037:GLN:HB3	1:D:1051:PHE:HZ	1.54	0.72
1:C:1037:GLN:HB3	1:D:1051:PHE:CZ	2.25	0.70
1:B:590:ASP:OD1	1:B:594:ARG:NH2	2.24	0.70
1:C:619:LEU:HD11	1:C:654:PHE:CD2	2.29	0.67
1:A:677:CYS:N	1:A:713:HIS:HD2	1.84	0.66
1:C:677:CYS:N	1:C:713:HIS:HD2	1.83	0.65
1:B:1051:PHE:CE1	1:B:1060:ARG:HD2	2.33	0.63
1:A:953:GLY:HA2	1:A:956:LEU:HD12	1.81	0.63
1:D:677:CYS:N	1:D:713:HIS:HD2	1.80	0.61
1:A:891[B]:MET:HE2	1:A:918:VAL:HG21	1.83	0.60
1:A:482:ASP:OD2	1:A:1066:ARG:NH2	2.35	0.60
1:C:667:MET:HA	1:C:670:ILE:HD12	1.84	0.59
1:A:1032:LEU:HA	1:A:1055:ASN:HD21	1.67	0.59
1:C:694:LYS:HG2	1:C:695:TYR:CE2	2.38	0.59
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.68	0.58
1:A:753:GLY:HA3	1:A:831:PRO:HB3	1.85	0.58
1:C:566:ARG:CG	1:C:566:ARG:HH11	2.16	0.58
1:C:775:ASP:HB2	1:C:811:SER:OG	2.04	0.57
1:A:974:ARG:HH12	1:A:980:GLU:CD	2.13	0.56
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.71	0.56
1:D:617:GLN:HG3	1:D:650:LEU:HB3	1.88	0.56
1:C:1051:PHE:CZ	1:D:1037:GLN:HB3	2.41	0.55
1:B:754:ILE:HG22	1:D:756:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:MET:HE2	1:B:918:VAL:HG21	1.89	0.55
1:C:716:ALA:HA	1:C:745:HIS:O	2.07	0.55
1:B:617:GLN:HG3	1:B:650:LEU:HD22	1.88	0.55
1:A:851:GLN:O	1:A:854:SER:HB2	2.07	0.54
1:A:566:ARG:CG	1:A:566:ARG:HH11	2.20	0.54
1:A:1026:ILE:HD13	1:A:1026:ILE:O	2.07	0.54
1:B:566:ARG:HH11	1:B:566:ARG:HG3	1.72	0.54
1:C:664:ARG:HH22	1:C:710:ALA:HA	1.73	0.54
1:A:566:ARG:HH11	1:A:566:ARG:HG3	1.74	0.53
1:C:909:ASP:O	1:C:910:ARG:C	2.51	0.53
1:B:1003:PRO:O	1:B:1006:VAL:HG22	2.08	0.53
1:A:901:THR:O	1:A:904:ASP:HB2	2.09	0.53
1:B:915:PRO:O	1:B:919:VAL:HG23	2.09	0.53
1:A:518:THR:HB	1:A:615:LEU:HG	1.92	0.52
1:B:566:ARG:HH11	1:B:566:ARG:CG	2.22	0.52
1:B:621:ARG:CB	1:B:624:ASN:OD1	2.57	0.52
1:D:566:ARG:HH11	1:D:566:ARG:CG	2.22	0.52
1:C:617:GLN:HG3	1:C:650:LEU:HB3	1.92	0.52
1:B:657:LEU:HA	1:B:879:VAL:CG1	2.40	0.52
1:C:566:ARG:CG	1:C:566:ARG:NH1	2.73	0.52
1:B:756:ALA:CB	1:D:754:ILE:HG22	2.40	0.52
1:B:851:GLN:O	1:B:854:SER:HB2	2.10	0.52
1:A:633:ASP:N	1:A:633:ASP:OD1	2.44	0.51
1:C:1038:ALA:HB1	1:D:1038:ALA:HB1	1.94	0.50
1:A:617:GLN:HG3	1:A:650:LEU:HB3	1.93	0.50
1:D:551:HIS:CE1	1:D:559:MET:HB3	2.47	0.50
1:C:566:ARG:HH11	1:C:566:ARG:HG3	1.76	0.50
1:D:566:ARG:HH11	1:D:566:ARG:HG3	1.76	0.50
1:B:726:PRO:HG2	1:D:760:LEU:HD13	1.94	0.49
1:D:590:ASP:HB2	1:D:987:TYR:CZ	2.48	0.49
1:B:746:PHE:HB3	1:B:770:VAL:HG12	1.95	0.48
1:C:664:ARG:CG	1:C:664:ARG:NH1	2.55	0.48
1:C:1051:PHE:HZ	1:D:1037:GLN:HB3	1.78	0.48
1:A:518:THR:HG21	1:A:579:LEU:HD12	1.95	0.48
1:A:537:GLU:HG3	1:A:539:ARG:HG2	1.94	0.48
1:C:851:GLN:O	1:C:854:SER:HB2	2.14	0.48
1:A:1032:LEU:HA	1:A:1055:ASN:ND2	2.29	0.48
1:A:482:ASP:CG	1:A:1066:ARG:HH21	2.21	0.48
1:C:548:ARG:HD2	1:C:548:ARG:C	2.38	0.48
1:A:555:LEU:HD11	1:A:818:ARG:HG3	1.95	0.47
1:B:549:ASP:HB3	1:B:783:GLN:HE22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:ARG:NH1	1:B:975:GLU:O	2.45	0.47
1:D:518:THR:HB	1:D:615:LEU:HG	1.94	0.47
1:C:555:LEU:HD11	1:C:818:ARG:HG3	1.95	0.47
1:B:757:ALA:HB2	1:D:757:ALA:HA	1.95	0.47
1:D:555:LEU:HD11	1:D:818:ARG:HG3	1.96	0.47
1:B:608:ARG:HA	1:B:616:LEU:HD11	1.96	0.47
1:B:942:LEU:HD13	1:B:945:GLU:O	2.15	0.47
1:C:750:ASP:C	1:C:780:ASN:O	2.58	0.47
1:A:1003:PRO:O	1:A:1006:VAL:HG22	2.15	0.47
1:D:753:GLY:HA3	1:D:831:PRO:HB3	1.97	0.47
1:D:929:PRO:HD3	1:D:933:TRP:CZ2	2.49	0.47
1:A:566:ARG:CG	1:A:566:ARG:NH1	2.78	0.46
1:B:754:ILE:HG22	1:D:756:ALA:HB1	1.97	0.46
1:C:706:GLU:OE1	1:C:706:GLU:HA	2.12	0.46
1:B:757:ALA:HA	1:D:757:ALA:HB2	1.96	0.46
1:A:617:GLN:HG3	1:A:650:LEU:HD22	1.97	0.46
1:B:753:GLY:HA3	1:B:831:PRO:HB3	1.96	0.46
1:A:591:VAL:HG13	1:A:595:PHE:HD2	1.81	0.46
1:C:664:ARG:HH11	1:C:664:ARG:HG2	1.77	0.46
1:D:844:GLN:O	1:D:844:GLN:CG	2.63	0.46
1:C:551:HIS:CE1	1:C:559:MET:HB3	2.50	0.46
1:C:557:THR:HG21	1:C:587:ALA:HB3	1.98	0.46
1:A:929:PRO:HD3	1:A:933:TRP:CZ2	2.51	0.46
1:A:872:ASN:HB2	1:A:880:LYS:HD3	1.97	0.45
1:D:486:ASN:HD21	1:D:1066:ARG:H	1.63	0.45
1:A:942:LEU:HA	1:A:942:LEU:HD23	1.68	0.45
1:D:566:ARG:CG	1:D:566:ARG:NH1	2.79	0.45
1:C:793:LEU:HA	1:C:793:LEU:HD23	1.74	0.45
1:A:891[B]:MET:HE1	1:A:914:PHE:CD1	2.52	0.45
1:C:753:GLY:HA3	1:C:831:PRO:HB3	1.98	0.45
1:A:720:MET:HG3	1:A:881:VAL:HG23	1.98	0.45
1:A:968:ILE:HD13	1:A:984:TYR:CD1	2.52	0.45
1:A:882:THR:HA	1:A:883:PRO:HA	1.73	0.44
1:B:566:ARG:CG	1:B:566:ARG:NH1	2.79	0.44
1:A:548:ARG:NH2	1:A:552:GLN:OE1	2.49	0.44
1:B:551:HIS:CE1	1:B:559:MET:HB3	2.52	0.44
1:C:664:ARG:NH2	1:C:710:ALA:HA	2.32	0.44
1:C:929:PRO:HD3	1:C:933:TRP:CZ2	2.53	0.44
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.78	0.43
1:B:617:GLN:HG3	1:B:650:LEU:HB3	2.00	0.43
1:B:961:LEU:HD23	1:B:961:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:TYR:C	1:A:948:TYR:CD1	2.96	0.43
1:B:555:LEU:HD11	1:B:818:ARG:HG3	2.01	0.43
1:C:486:ASN:HD21	1:C:1066:ARG:H	1.65	0.43
1:A:833:SER:C	1:A:835:VAL:H	2.26	0.43
1:C:963:ALA:O	1:C:967:VAL:HG23	2.19	0.43
1:D:557:THR:HG21	1:D:587:ALA:HB3	2.01	0.43
1:B:942:LEU:HD23	1:B:942:LEU:HA	1.78	0.43
1:D:882:THR:HA	1:D:883:PRO:HA	1.76	0.43
1:C:715:ILE:O	1:C:744:ILE:HA	2.19	0.42
1:D:804:PRO:HA	1:D:807:ILE:HD12	2.00	0.42
1:A:544:ASP:OD1	1:A:544:ASP:C	2.62	0.42
1:A:551:HIS:CE1	1:A:559:MET:HB3	2.54	0.42
1:A:716:ALA:HA	1:A:745:HIS:O	2.20	0.42
1:B:683:TYR:O	1:B:720:MET:HE1	2.19	0.42
1:A:1027:GLU:O	1:A:1028:LYS:C	2.62	0.42
1:B:833:SER:HB3	1:D:788:SER:N	2.33	0.42
1:B:882:THR:HA	1:B:883:PRO:HA	1.76	0.42
1:C:882:THR:HA	1:C:883:PRO:HA	1.75	0.42
1:D:608:ARG:HA	1:D:616:LEU:HD11	2.02	0.42
1:B:723:LEU:HD11	1:B:839:GLU:HG2	2.01	0.41
1:A:833:SER:C	1:A:835:VAL:N	2.74	0.41
1:B:1061:ILE:HD13	1:B:1061:ILE:HA	1.76	0.41
1:C:474:THR:HG23	1:C:1059:ARG:NH2	2.34	0.41
1:C:548:ARG:NH2	1:C:552:GLN:OE1	2.53	0.41
1:B:929:PRO:HD3	1:B:933:TRP:CZ2	2.55	0.41
1:C:872:ASN:HB2	1:C:880:LYS:HD3	2.01	0.41
1:D:745:HIS:HA	1:D:769:ALA:O	2.20	0.41
1:D:853:ARG:HG3	1:D:854:SER:N	2.35	0.41
1:D:1023:PHE:CD1	1:D:1033:VAL:HG22	2.55	0.41
1:A:657:LEU:HD23	1:A:657:LEU:HA	1.90	0.41
1:A:750:ASP:C	1:A:780:ASN:O	2.63	0.41
1:B:835:VAL:HA	1:B:838:HIS:CE1	2.56	0.41
1:D:922:LEU:O	1:D:938:GLN:NE2	2.54	0.41
1:B:844:GLN:O	1:B:844:GLN:CG	2.67	0.41
1:B:1027:GLU:O	1:B:1028:LYS:C	2.63	0.41
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.85	0.41
1:A:556:ALA:O	1:A:558:ARG:HD3	2.21	0.41
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.94	0.41
1:C:638:TYR:O	1:C:642:GLN:HG2	2.21	0.41
1:C:840:MET:HE2	1:C:848:LEU:CD2	2.50	0.41
1:D:486:ASN:ND2	1:D:1066:ARG:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:TYR:O	1:D:642:GLN:HG2	2.21	0.41
1:D:844:GLN:O	1:D:844:GLN:HG2	2.19	0.41
1:A:835:VAL:HA	1:A:838:HIS:CE1	2.56	0.41
1:C:518:THR:HB	1:C:615:LEU:HG	2.03	0.41
1:C:779:GLY:O	1:C:780:ASN:C	2.63	0.41
1:D:537:GLU:HG3	1:D:539:ARG:HG2	2.03	0.41
1:B:649:ASP:HA	1:B:675:LYS:HD2	2.01	0.40
1:D:827:ASP:C	1:D:827:ASP:OD1	2.64	0.40
1:D:1027:GLU:O	1:D:1028:LYS:C	2.63	0.40
1:C:544:ASP:OD1	1:C:544:ASP:C	2.65	0.40
1:C:603:ARG:O	1:C:607:ILE:HG13	2.22	0.40
1:A:608:ARG:HA	1:A:616:LEU:HD11	2.03	0.40
1:D:518:THR:HG21	1:D:579:LEU:HD12	2.04	0.40
1:B:521:LEU:HD23	1:B:521:LEU:HA	1.96	0.40
1:D:549:ASP:HB3	1:D:783:GLN:NE2	2.36	0.40

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)
1:A:512:ASN:O	1:D:516:ASP:OD2[3_344]	1.76	0.44

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	595/632 (94%)	559 (94%)	31 (5%)	5 (1%)	16 47
1	B	590/632 (93%)	555 (94%)	31 (5%)	4 (1%)	18 50
1	C	590/632 (93%)	554 (94%)	35 (6%)	1 (0%)	43 73
1	D	585/632 (93%)	554 (95%)	29 (5%)	2 (0%)	36 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2360/2528 (93%)	2222 (94%)	126 (5%)	12 (0%)	24	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1028	LYS
1	B	1028	LYS
1	C	1028	LYS
1	D	1028	LYS
1	A	500	ASN
1	D	500	ASN
1	B	512	ASN
1	A	510	ASN
1	A	511	GLY
1	A	845	PHE
1	B	500	ASN
1	B	822	ALA

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	443/519 (85%)	421 (95%)	22 (5%)	22	54
1	B	398/519 (77%)	375 (94%)	23 (6%)	18	49
1	C	406/519 (78%)	382 (94%)	24 (6%)	18	48
1	D	349/519 (67%)	338 (97%)	11 (3%)	34	65
All	All	1596/2076 (77%)	1516 (95%)	80 (5%)	22	54

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	518	THR
1	A	524	THR

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Mol	Chain	Res	Type
1	A	557	THR
1	A	566	ARG
1	A	577	ASN
1	A	584	TRP
1	A	590	ASP
1	A	597	THR
1	A	633	ASP
1	A	666	SER
1	A	672	GLU
1	A	720	MET
1	A	737	ARG
1	A	794	SER
1	A	860	ARG
1	A	882	THR
1	A	910	ARG
1	A	943	LYS
1	A	967	VAL
1	A	998	SER
1	A	1026	ILE
1	B	476	LEU
1	B	510	ASN
1	B	518	THR
1	B	524	THR
1	B	557	THR
1	B	566	ARG
1	B	584	TRP
1	B	590	ASP
1	B	597	THR
1	B	624	ASN
1	B	626	VAL
1	B	661	GLU
1	B	666	SER
1	B	692	ARG
1	B	720	MET
1	B	794	SER
1	B	855	LEU
1	B	879	VAL
1	B	882	THR
1	B	899	ASP
1	B	926	LEU
1	B	989	LYS
1	B	1044	SER

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Mol	Chain	Res	Type
1	C	508	TYR
1	C	518	THR
1	C	524	THR
1	C	542	LEU
1	C	557	THR
1	C	566	ARG
1	C	577	ASN
1	C	584	TRP
1	C	590	ASP
1	C	597	THR
1	C	661	GLU
1	C	664	ARG
1	C	703	LEU
1	C	706	GLU
1	C	720	MET
1	C	794	SER
1	C	809	ARG
1	C	860	ARG
1	C	882	THR
1	C	886	LYS
1	C	910	ARG
1	C	931	SER
1	C	998	SER
1	C	999	ASP
1	D	518	THR
1	D	524	THR
1	D	557	THR
1	D	577	ASN
1	D	590	ASP
1	D	597	THR
1	D	720	MET
1	D	794	SER
1	D	863	GLN
1	D	882	THR
1	D	998	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	630	ASN
1	A	713	HIS

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Mol	Chain	Res	Type
1	A	783	GLN
1	A	820	GLN
1	A	1055	ASN
1	B	486	ASN
1	B	630	ASN
1	B	713	HIS
1	B	783	GLN
1	C	486	ASN
1	C	577	ASN
1	C	630	ASN
1	C	713	HIS
1	C	783	GLN
1	C	872	ASN
1	C	1037	GLN
1	D	486	ASN
1	D	630	ASN
1	D	713	HIS
1	D	783	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	KCX	C	718	1,2	10,11,12	0.85	0	6,12,14	7.73	2 (33%)
1	KCX	B	718	1,2	10,11,12	0.55	0	6,12,14	3.58	2 (33%)
1	KCX	D	718	1,2	10,11,12	0.69	0	6,12,14	2.59	1 (16%)
1	KCX	A	718	1,2	10,11,12	0.44	0	6,12,14	3.88	3 (50%)

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
1	KCX	C	718	1,2	-	2/9/10/12	-
1	KCX	B	718	1,2	-	1/9/10/12	-
1	KCX	D	718	1,2	-	1/9/10/12	-
1	KCX	A	718	1,2	-	1/9/10/12	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	718	KCX	CE-NZ-CX	16.97	150.78	121.98
1	C	718	KCX	OQ1-CX-NZ	-8.26	112.38	124.92
1	A	718	KCX	CE-NZ-CX	8.23	135.95	121.98
1	B	718	KCX	CE-NZ-CX	7.95	135.47	121.98
1	D	718	KCX	CE-NZ-CX	6.00	132.17	121.98
1	A	718	KCX	OQ1-CX-NZ	3.25	129.86	124.92
1	A	718	KCX	CD-CE-NZ	3.15	121.02	112.20
1	B	718	KCX	CD-CE-NZ	2.94	120.44	112.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718	KCX	O-C-CA-CB
1	B	718	KCX	O-C-CA-CB
1	C	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB
1	C	718	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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

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	596/632 (94%)	-0.28	7 (1%) 76 59	30, 65, 95, 159	20 (3%)
1	B	594/632 (93%)	0.23	30 (5%) 33 20	45, 89, 156, 239	13 (2%)
1	C	594/632 (93%)	0.17	22 (3%) 45 28	39, 90, 166, 216	20 (3%)
1	D	593/632 (93%)	0.76	59 (9%) 13 8	73, 111, 155, 195	12 (2%)
All	All	2377/2528 (94%)	0.22	118 (4%) 34 20	30, 88, 154, 239	65 (2%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	875	PHE	4.7
1	B	874	MET	4.3
1	D	676	LEU	4.0
1	C	509	ALA	3.9
1	D	509	ALA	3.9
1	C	685	GLY	3.7
1	D	648	ILE	3.6
1	D	839	GLU	3.6
1	C	1055	ASN	3.6
1	D	885	SER	3.5
1	B	871	ALA	3.5
1	B	864	VAL	3.5
1	D	476	LEU	3.5
1	D	1003	PRO	3.4
1	B	585	GLY	3.3
1	D	513	GLY	3.3
1	C	639	PHE	3.3
1	C	1037	GLN	3.2
1	C	1045	GLN	3.2
1	D	937	LEU	3.1
1	C	500	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	674	ASN	3.0
1	D	542	LEU	3.0
1	B	892	ALA	3.0
1	D	512	ASN	2.9
1	D	707	LEU	2.9
1	D	625	GLY	2.9
1	D	843	GLY	2.9
1	D	721	ALA	2.9
1	D	1027	GLU	2.9
1	C	634	ASN	2.9
1	B	875	PHE	2.8
1	D	879	VAL	2.8
1	C	899	ASP	2.8
1	D	619	LEU	2.8
1	D	844	GLN	2.8
1	B	905	VAL	2.8
1	B	911	GLU	2.8
1	D	630	ASN	2.8
1	D	941	ALA	2.7
1	C	1026	ILE	2.7
1	D	715	ILE	2.7
1	D	906	VAL	2.7
1	B	696	ASP	2.7
1	C	919	VAL	2.7
1	D	921	MET	2.6
1	D	756	ALA	2.6
1	A	512	ASN	2.6
1	B	630	ASN	2.6
1	C	510	ASN	2.6
1	D	624	ASN	2.6
1	C	1044	SER	2.6
1	A	1026	ILE	2.6
1	D	706	GLU	2.6
1	D	968	ILE	2.6
1	B	721	ALA	2.6
1	B	880	LYS	2.6
1	D	1028	LYS	2.6
1	B	863	GLN	2.6
1	D	661	GLU	2.6
1	B	509	ALA	2.6
1	B	896	VAL	2.5
1	D	723	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	623	ALA	2.5
1	C	659	TRP	2.5
1	B	908	PRO	2.5
1	C	902	VAL	2.5
1	D	700	TYR	2.5
1	B	827	ASP	2.4
1	D	681	ILE	2.4
1	B	791	GLU	2.4
1	B	914	PHE	2.4
1	B	872	ASN	2.4
1	B	919	VAL	2.4
1	D	683	TYR	2.4
1	D	713	HIS	2.4
1	B	867	ALA	2.4
1	A	511	GLY	2.3
1	C	638	TYR	2.3
1	A	510	ASN	2.3
1	B	512	ASN	2.3
1	A	595	PHE	2.3
1	B	904	ASP	2.3
1	D	840	MET	2.3
1	A	577	ASN	2.3
1	B	661	GLU	2.3
1	D	769	ALA	2.3
1	C	656	CYS	2.3
1	D	1037	GLN	2.3
1	D	510	ASN	2.3
1	D	1013	PHE	2.3
1	D	989	LYS	2.3
1	D	1061	ILE	2.3
1	C	621	ARG	2.3
1	D	976	VAL	2.3
1	D	664	ARG	2.2
1	D	791	GLU	2.2
1	D	950	VAL	2.2
1	D	728	ALA	2.2
1	D	919	VAL	2.2
1	B	722	GLY	2.2
1	D	957	LYS	2.2
1	D	926	LEU	2.2
1	D	961	LEU	2.2
1	B	693	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	990	VAL	2.1
1	C	960	ASP	2.1
1	B	941	ALA	2.1
1	A	766	GLY	2.1
1	B	700	TYR	2.1
1	D	1039	VAL	2.1
1	B	868	TYR	2.1
1	D	631	TYR	2.1
1	D	514	VAL	2.0
1	C	893	LEU	2.0
1	C	511	GLY	2.0
1	D	665	VAL	2.0
1	C	875	PHE	2.0

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
1	KCX	D	718	12/13	0.89	0.18	93,96,98,99	0
1	KCX	B	718	12/13	0.92	0.12	78,81,91,93	0
1	KCX	A	718	12/13	0.95	0.08	51,54,60,66	0
1	KCX	C	718	12/13	0.96	0.11	72,75,85,86	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
3	CL	A	1102	1/1	0.96	0.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	C	1102	1/1	0.96	0.04	86,86,86,86	0
2	ZN	C	1101	1/1	0.99	0.03	69,69,69,69	0
2	ZN	A	1101	1/1	0.99	0.03	58,58,58,58	0
2	ZN	B	1101	1/1	0.99	0.03	77,77,77,77	0
2	ZN	D	1101	1/1	1.00	0.02	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.