



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:10 PM EDT

PDB ID : 7EIY / pdb_00007eiy
Title : Human histidine decarboxylase mutant Y334F soaking with histidine
Authors : Komori, H.
Deposited on : 2021-04-01
Resolution : 2.20 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

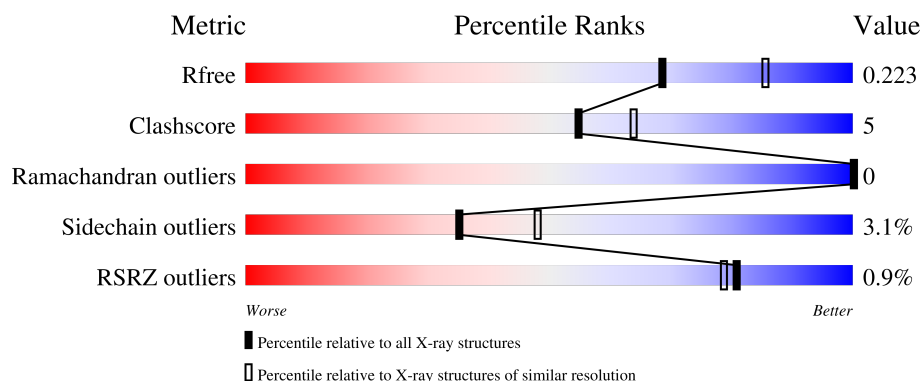
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	481	
1	B	481	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7731 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 Histidine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	3	0
			3731	2390	639	679	23			
1	B	466	Total	C	N	O	S	0	0	0
			3711	2374	636	678	23			

There are 14 discrepancies between the modelled and reference sequences:

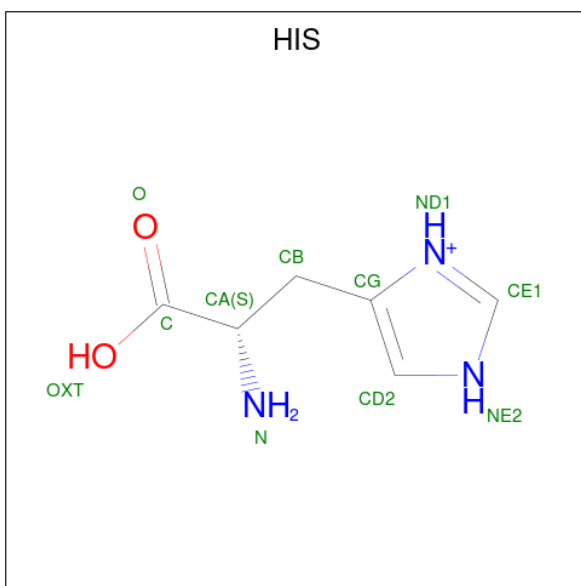
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P19113
A	-2	PRO	-	expression tag	UNP P19113
A	-1	LEU	-	expression tag	UNP P19113
A	0	GLY	-	expression tag	UNP P19113
A	1	SER	-	expression tag	UNP P19113
A	180	SER	CYS	engineered mutation	UNP P19113
A	418	SER	CYS	engineered mutation	UNP P19113
B	-3	GLY	-	expression tag	UNP P19113
B	-2	PRO	-	expression tag	UNP P19113
B	-1	LEU	-	expression tag	UNP P19113
B	0	GLY	-	expression tag	UNP P19113
B	1	SER	-	expression tag	UNP P19113
B	180	SER	CYS	engineered mutation	UNP P19113
B	418	SER	CYS	engineered mutation	UNP P19113

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is HISTIDINE (CCD ID: HIS) (formula: $C_6H_{10}N_3O_2$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

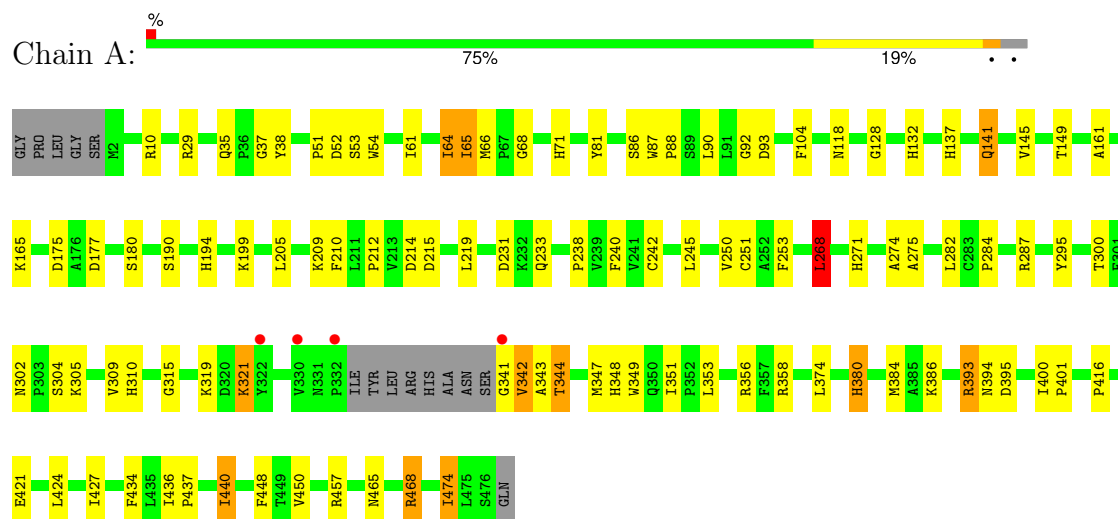
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		
5	B	96	Total	O	0	0
			96	96		

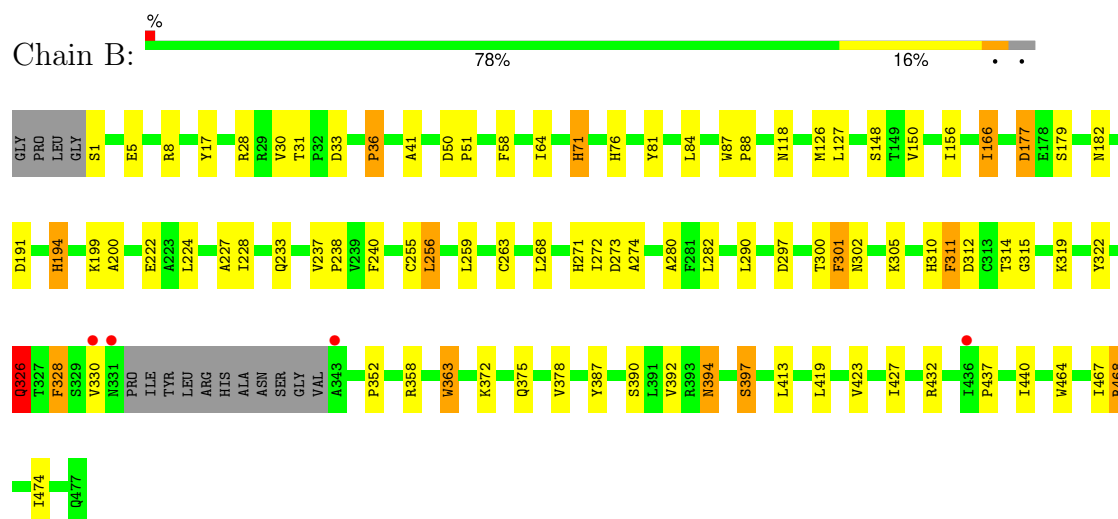
3 Residue-property plots

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: Histidine decarboxylase



• Molecule 1: Histidine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.93Å 85.00Å 187.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.43 – 2.20 36.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.43-2.20) 99.9 (36.43-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.167 , 0.224 0.173 , 0.223	Depositor DCC
R_{free} test set	2425 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7731	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: CSX, PLP, 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	1.43	33/3827 (0.9%)	1.56	34/5189 (0.7%)
1	B	1.36	14/3797 (0.4%)	1.59	27/5146 (0.5%)
All	All	1.40	47/7624 (0.6%)	1.57	61/10335 (0.6%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	HIS	CE1-NE2	10.43	1.43	1.32
1	B	310	HIS	CE1-NE2	8.78	1.41	1.32
1	A	245	LEU	C-O	7.85	1.33	1.23
1	A	448	PHE	C-O	7.62	1.32	1.24
1	B	71	HIS	CE1-NE2	7.59	1.40	1.32
1	A	393[A]	ARG	C-O	-7.46	1.14	1.24
1	A	393[B]	ARG	C-O	-7.46	1.14	1.24
1	A	251	CYS	C-O	7.32	1.33	1.23
1	B	36	PRO	C-O	-7.26	1.13	1.23
1	A	52	ASP	C-O	-7.19	1.15	1.23
1	A	51	PRO	C-O	-6.92	1.15	1.23
1	B	238	PRO	C-O	-6.91	1.15	1.23
1	A	53	SER	C-O	6.74	1.32	1.23
1	A	394	ASN	C-O	-6.56	1.15	1.24
1	A	145	VAL	C-O	6.54	1.30	1.23
1	A	65	ILE	C-O	6.47	1.31	1.24
1	A	284	PRO	C-O	-6.39	1.16	1.24
1	B	194	HIS	CE1-NE2	6.20	1.38	1.32
1	A	71	HIS	C-O	6.07	1.30	1.23
1	A	474	ILE	C-O	-6.02	1.16	1.24
1	B	148	SER	CA-CB	-5.97	1.44	1.53
1	A	380	HIS	CE1-NE2	5.94	1.38	1.32
1	A	66	MET	C-O	-5.91	1.19	1.24
1	B	271	HIS	C-O	5.91	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	TYR	C-O	-5.70	1.16	1.24
1	A	194	HIS	CE1-NE2	5.59	1.38	1.32
1	A	205	LEU	C-O	-5.55	1.15	1.23
1	A	342	VAL	N-CA	5.46	1.52	1.46
1	A	68	GLY	C-O	5.41	1.28	1.24
1	A	424	LEU	C-O	5.39	1.30	1.24
1	A	29	ARG	C-O	-5.39	1.17	1.24
1	A	212	PRO	C-O	5.38	1.30	1.23
1	A	128	GLY	C-O	-5.36	1.16	1.24
1	A	450	VAL	C-O	5.32	1.30	1.24
1	B	301	PHE	C-O	-5.28	1.17	1.23
1	B	64	ILE	N-CA	5.27	1.50	1.46
1	B	387	TYR	C-O	5.23	1.30	1.24
1	A	268	LEU	C-O	5.22	1.30	1.24
1	B	84	LEU	C-O	5.21	1.30	1.24
1	A	137	HIS	CE1-NE2	5.19	1.37	1.32
1	A	214	ASP	C-O	5.19	1.29	1.23
1	A	401	PRO	C-O	-5.18	1.17	1.24
1	B	17	TYR	C-O	5.16	1.30	1.24
1	A	92	GLY	C-O	5.12	1.30	1.23
1	A	104	PHE	C-O	5.08	1.30	1.24
1	B	118	ASN	C-O	5.07	1.30	1.24
1	B	41	ALA	C-O	-5.07	1.17	1.24

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	GLY	CA-C-N	11.51	136.76	120.53
1	A	341	GLY	C-N-CA	11.51	136.76	120.53
1	A	81	TYR	CB-CA-C	7.97	121.28	109.08
1	B	328	PHE	CB-CA-C	-7.01	97.70	109.75
1	B	312	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	374	LEU	N-CA-C	-6.88	103.86	111.36
1	A	240	PHE	CA-CB-CG	6.57	120.36	113.80
1	B	81	TYR	CB-CA-C	6.53	118.96	109.09
1	B	394	ASN	CA-CB-CG	-6.43	106.17	112.60
1	B	358	ARG	CB-CG-CD	-6.38	96.64	111.30
1	A	395	ASP	CB-CA-C	6.36	116.47	110.17
1	B	150	VAL	CA-C-O	-6.21	114.58	121.17
1	A	37	GLY	CA-C-N	6.21	128.89	120.38
1	A	37	GLY	C-N-CA	6.21	128.89	120.38
1	B	326	GLN	N-CA-CB	6.07	120.46	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ASP	CA-CB-CG	-6.04	106.56	112.60
1	B	200	ALA	CA-C-N	6.00	126.60	119.94
1	B	200	ALA	C-N-CA	6.00	126.60	119.94
1	A	210	PHE	CA-CB-CG	-5.97	107.83	113.80
1	B	58	PHE	CA-C-O	-5.95	114.57	120.82
1	A	64	ILE	CA-C-O	-5.94	113.35	120.78
1	B	166	ILE	CA-C-O	-5.94	114.77	120.95
1	B	191	ASP	N-CA-C	-5.92	106.15	113.19
1	A	342	VAL	N-CA-C	5.88	117.33	110.62
1	A	465	ASN	CA-C-O	-5.83	114.37	120.55
1	B	375	GLN	CA-C-O	-5.79	114.70	120.90
1	A	342	VAL	CA-C-O	-5.70	115.13	121.05
1	A	400	ILE	CB-CA-C	5.65	116.45	111.08
1	A	416	PRO	CA-C-N	5.61	128.06	120.38
1	A	416	PRO	C-N-CA	5.61	128.06	120.38
1	B	233	GLN	CB-CA-C	5.49	119.90	110.79
1	A	209	LYS	CB-CA-C	5.49	119.27	110.16
1	A	253	PHE	CA-CB-CG	-5.46	108.34	113.80
1	B	358	ARG	CG-CD-NE	5.44	123.97	112.00
1	B	363	TRP	CA-C-O	-5.43	115.11	120.82
1	A	287	ARG	CA-C-O	-5.40	112.75	119.18
1	A	214	ASP	CA-C-N	5.39	128.05	120.28
1	A	214	ASP	C-N-CA	5.39	128.05	120.28
1	B	437	PRO	CA-C-O	-5.38	115.21	121.34
1	B	237	VAL	CA-C-O	-5.34	117.25	120.88
1	A	61	ILE	N-CA-C	-5.33	105.41	110.42
1	A	386	LYS	N-CA-CB	-5.31	102.30	110.16
1	A	118	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	427	ILE	CA-C-N	5.29	127.90	120.28
1	A	427	ILE	C-N-CA	5.29	127.90	120.28
1	A	161	ALA	CA-C-O	-5.24	115.31	120.82
1	B	311	PHE	CA-C-N	5.24	131.13	121.70
1	B	311	PHE	C-N-CA	5.24	131.13	121.70
1	A	215	ASP	CA-C-O	-5.24	114.18	120.10
1	B	240	PHE	CA-CB-CG	5.24	119.03	113.80
1	A	231	ASP	CA-C-O	-5.23	114.88	120.42
1	A	440	ILE	O-C-N	5.20	127.76	122.71
1	A	358	ARG	CG-CD-NE	5.17	123.38	112.00
1	A	421	GLU	N-CA-CB	5.15	117.62	109.94
1	B	314	THR	CA-CB-OG1	-5.14	101.89	109.60
1	B	227	ALA	CA-C-N	5.12	127.00	120.56
1	B	227	ALA	C-N-CA	5.12	127.00	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	HIS	CA-C-N	5.04	125.69	119.99
1	A	380	HIS	C-N-CA	5.04	125.69	119.99
1	B	33	ASP	CA-C-O	-5.01	116.60	122.37
1	B	319	LYS	O-C-N	5.01	128.74	122.23

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	3731	0	3701	38	0
1	B	3711	0	3672	41	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	11	0	6	0	0
3	B	11	0	6	0	0
4	A	5	0	0	0	0
5	A	136	0	0	0	0
5	B	96	0	0	1	0
All	All	7731	0	7397	71	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (71) 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:10:ARG:HD2	1:A:54:TRP:CD1	2.14	0.82
1:A:468:ARG:O	1:A:468:ARG:HD3	1.91	0.71
1:B:256:LEU:HD11	1:B:272:ILE:HD11	1.75	0.68
1:B:256:LEU:HD11	1:B:272:ILE:CD1	2.28	0.63
1:B:87:TRP:HB2	1:B:88:PRO:HD3	1.82	0.61
1:A:434:PHE:CZ	1:A:436:ILE:HD11	2.35	0.60
1:A:87:TRP:HB2	1:A:88:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ILE:O	1:B:199:LYS:HE2	2.02	0.59
1:A:199:LYS:HE3	1:B:328:PHE:HB3	1.85	0.58
1:B:228:ILE:HD11	1:B:268:LEU:HD11	1.83	0.58
1:A:468:ARG:HD3	1:A:468:ARG:C	2.28	0.57
1:A:436:ILE:HG23	1:A:437:PRO:HD2	1.88	0.56
1:B:5:GLU:OE2	1:B:8:ARG:HD3	2.05	0.56
1:B:177:ASP:OD1	1:B:179:SER:N	2.38	0.56
1:B:322:TYR:O	1:B:326:GLN:HG2	2.08	0.53
1:A:10:ARG:CD	1:A:54:TRP:CD1	2.91	0.52
1:A:353:LEU:HD22	1:B:194:HIS:CE1	2.45	0.52
1:B:397:SER:OG	1:B:468:ARG:NH2	2.43	0.52
1:A:344[A]:THR:HG21	1:A:349:TRP:HE1	1.77	0.50
1:A:250:VAL:CG1	1:A:440:ILE:HG21	2.42	0.50
1:B:87:TRP:N	1:B:88:PRO:CD	2.75	0.50
1:A:238:PRO:HB2	1:A:268:LEU:HD21	1.94	0.49
1:A:190:SER:HB2	1:A:219:LEU:HB2	1.94	0.49
1:B:280:ALA:HA	1:B:378:VAL:HG11	1.94	0.49
1:A:436:ILE:CG2	1:A:437:PRO:HD2	2.44	0.48
1:A:141:GLN:O	1:A:321:LYS:HD2	2.14	0.48
1:A:393[B]:ARG:HG3	1:A:393[B]:ARG:HH11	1.79	0.48
1:A:132:HIS:CE1	1:A:319:LYS:HE3	2.49	0.48
1:B:300:THR:HA	1:B:315:GLY:O	2.14	0.47
1:B:432:ARG:HD3	1:B:432:ARG:HA	1.62	0.47
1:B:302:ASN:HD22	1:B:305:LYS:NZ	2.13	0.47
1:A:356:ARG:HB3	1:B:311:PHE:CD2	2.50	0.46
1:A:10:ARG:HD2	1:A:54:TRP:NE1	2.31	0.46
1:B:392:VAL:HG22	1:B:464:TRP:CZ3	2.51	0.46
1:B:419:LEU:O	1:B:423:VAL:HG23	2.16	0.46
1:B:30:VAL:HG21	1:B:76:HIS:HB2	1.98	0.46
1:B:263:CYS:HB3	1:B:268:LEU:O	2.17	0.45
1:A:302:ASN:HD22	1:A:305:LYS:NZ	2.14	0.45
1:B:30:VAL:CG2	1:B:76:HIS:HB2	2.46	0.45
1:B:256:LEU:HD12	1:B:256:LEU:HA	1.80	0.45
1:B:274:ALA:O	1:B:301:PHE:HB2	2.16	0.45
1:B:156:ILE:HD11	5:B:1159:HOH:O	2.17	0.45
1:B:273:ASP:C	1:B:273:ASP:OD1	2.59	0.45
1:B:427:ILE:HD11	1:B:467:ILE:HA	1.99	0.44
1:A:250:VAL:HG11	1:A:440:ILE:HG21	1.99	0.44
1:A:35:GLN:O	1:A:38:TYR:HB3	2.18	0.44
1:A:65:ILE:HD11	1:B:363:TRP:CZ3	2.53	0.43
1:B:224:LEU:HD22	1:B:259:LEU:HD22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:THR:HA	1:A:315:GLY:O	2.18	0.43
1:A:384:MET:HE1	1:A:457:ARG:HG3	2.00	0.43
1:B:126:MET:HB3	1:B:282:LEU:HD22	2.01	0.43
1:A:149:THR:HG21	1:B:352:PRO:HB2	2.01	0.42
1:A:304:SER:HA	1:A:309:VAL:O	2.19	0.42
1:B:228:ILE:CD1	1:B:268:LEU:HD11	2.49	0.42
1:A:274:ALA:O	1:A:275:ALA:C	2.62	0.42
1:A:380:HIS:CE1	1:A:384:MET:HE3	2.54	0.42
1:B:127:LEU:HD11	1:B:301:PHE:CE1	2.55	0.42
1:A:356:ARG:HB3	1:B:311:PHE:HD2	1.84	0.42
1:B:413:LEU:HD23	1:B:413:LEU:HA	1.89	0.42
1:A:343:ALA:HB3	1:B:36:PRO:HB3	2.01	0.42
1:A:344[A]:THR:HG21	1:A:349:TRP:NE1	2.35	0.42
1:A:177:ASP:HB3	1:A:180:SER:OG	2.21	0.41
1:A:347:MET:HE3	1:A:348:HIS:CE1	2.55	0.41
1:B:290:LEU:HD12	1:B:290:LEU:HA	1.87	0.41
1:B:166:ILE:HD11	1:B:182:ASN:HB2	2.01	0.41
1:B:390:SER:O	1:B:394:ASN:ND2	2.47	0.41
1:A:344[A]:THR:CG2	1:A:349:TRP:HE1	2.32	0.41
1:B:28:ARG:HD2	1:B:71:HIS:CE1	2.55	0.41
1:B:50:ASP:HB3	1:B:51:PRO:HD2	2.03	0.40
1:A:242:CYS:HA	1:A:271:HIS:O	2.21	0.40
1:A:86:SER:O	1:A:90:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/481 (97%)	447 (96%)	18 (4%)	0	100	100
1	B	461/481 (96%)	443 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	926/962 (96%)	890 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	405/413 (98%)	391 (96%)	14 (4%)	32	43
1	B	402/413 (97%)	390 (97%)	12 (3%)	36	49
All	All	807/826 (98%)	781 (97%)	26 (3%)	35	47

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	A	93	ASP
1	A	141	GLN
1	A	165	LYS
1	A	175	ASP
1	A	233	GLN
1	A	268	LEU
1	A	282	LEU
1	A	321	LYS
1	A	342	VAL
1	A	344[A]	THR
1	A	344[B]	THR
1	A	468	ARG
1	A	474	ILE
1	B	1	SER
1	B	31	THR
1	B	177	ASP
1	B	222	GLU
1	B	256	LEU
1	B	326	GLN

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Mol	Chain	Res	Type
1	B	330	VAL
1	B	372	LYS
1	B	397	SER
1	B	440	ILE
1	B	468	ARG
1	B	474	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	302	ASN
1	A	441	GLN
1	B	118	ASN
1	B	302	ASN
1	B	405	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	CSX	A	255	1	3,6,7	0.55	0	1,6,8	1.59	0
1	CSX	B	255	1	3,6,7	1.27	1 (33%)	1,6,8	1.71	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
1	CSX	A	255	1	-	0/2/5/7	-
1	CSX	B	255	1	-	0/2/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	CSX	O-C	2.19	1.28	1.20

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	HIS	B	1001	2	10,11,11	1.12	1 (10%)	10,14,14	0.94	0
4	SO4	A	503	-	4,4,4	0.18	0	6,6,6	0.18	0
3	HIS	A	502	2	10,11,11	1.09	1 (10%)	10,14,14	1.07	0
2	PLP	A	501	3	15,15,16	1.11	2 (13%)	21,22,23	0.89	0
2	PLP	B	1000	3	15,15,16	1.25	1 (6%)	21,22,23	1.22	2 (9%)

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	HIS	B	1001	2	-	2/8/8/8	0/1/1/1
3	HIS	A	502	2	-	1/8/8/8	0/1/1/1
2	PLP	A	501	3	-	2/6/6/8	0/1/1/1
2	PLP	B	1000	3	-	2/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	PLP	C3-C2	3.95	1.45	1.41
3	B	1001	HIS	OXT-C	-2.91	1.21	1.30
2	A	501	PLP	C4A-C4	-2.50	1.46	1.51
3	A	502	HIS	OXT-C	-2.48	1.22	1.30
2	A	501	PLP	C3-C2	2.32	1.43	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	PLP	C4A-C4-C5	3.31	124.35	120.94
2	B	1000	PLP	O4P-C5A-C5	2.11	113.31	109.36

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1000	PLP	C5A-O4P-P-O1P
2	B	1000	PLP	C5A-O4P-P-O2P
2	A	501	PLP	C4-C5-C5A-O4P
2	A	501	PLP	C6-C5-C5A-O4P
3	B	1001	HIS	OXT-C-CA-N
3	A	502	HIS	OXT-C-CA-N
3	B	1001	HIS	O-C-CA-N

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	466/481 (96%)	-0.54	4 (0%) 81 79	16, 29, 52, 72	3 (0%)
1	B	465/481 (96%)	-0.34	4 (0%) 81 79	21, 40, 64, 88	0
All	All	931/962 (96%)	-0.44	8 (0%) 81 79	16, 33, 61, 88	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	GLY	3.2
1	B	436	ILE	3.2
1	B	331	ASN	2.5
1	A	330	VAL	2.5
1	A	332	PRO	2.2
1	A	322	TYR	2.2
1	B	330	VAL	2.1
1	B	343	ALA	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	CSX	B	255	7/8	0.94	0.06	54,57,64,66	0
1	CSX	A	255	7/8	0.96	0.06	28,32,42,48	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($\text{\AA}^2$)	Q<0.9
3	HIS	B	1001	11/11	0.94	0.07	35,37,42,44	0
4	SO4	A	503	5/5	0.95	0.10	41,45,52,62	0
3	HIS	A	502	11/11	0.96	0.07	25,26,30,31	0
2	PLP	B	1000	15/16	0.97	0.06	31,38,43,44	0
2	PLP	A	501	15/16	0.98	0.05	24,26,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.