



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:18 PM EDT

PDB ID : 3AYZ / pdb_00003ayz
Title : Membrane-bound respiratory [NiFe] hydrogenase from *Hydrogenovibrio marinus* in an air-oxidized condition
Authors : Shomura, Y.; Yoon, K.S.; Nishihara, H.; Higuchi, Y.
Deposited on : 2011-05-20
Resolution : 1.22 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

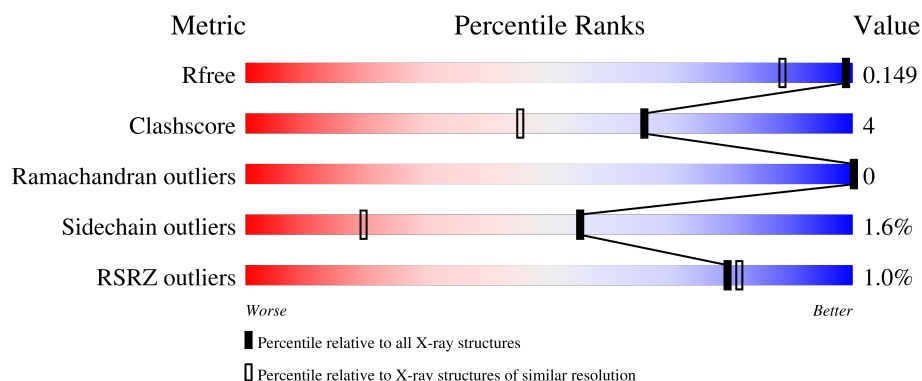
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.22 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	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (1.24-1.20)

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	596	 87% 11% •
1	C	596	 87% 11% •
2	B	283	 80% 15% • •
2	D	283	 78% 14% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	O	A	607	-	-	X	-
7	O	C	607	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 15529 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 Membrane-bound hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	19	0
			4770	3030	831	884	25			
1	C	595	Total	C	N	O	S	0	15	0
			4750	3014	829	882	25			

- Molecule 2 is a protein called Membrane-bound hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	273	Total	C	N	O	S	0	8	0
			2159	1370	369	399	21			
2	D	267	Total	C	N	O	S	0	8	0
			2109	1341	358	390	20			

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 4 is NICKEL (III) ION (CCD ID: 3NI) (formula: Ni).

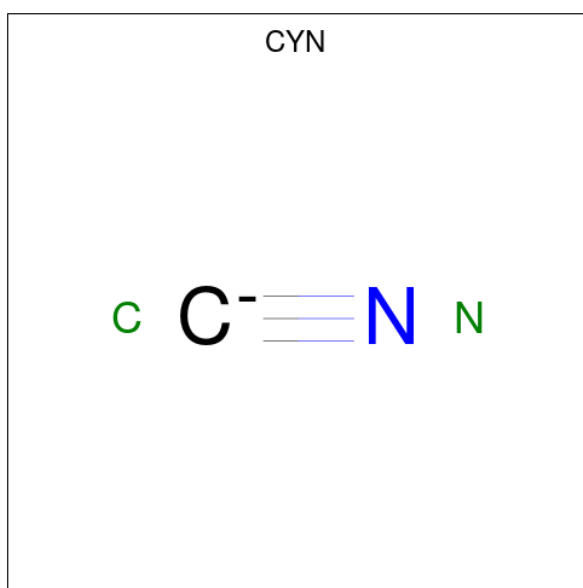
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		

- Molecule 5 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 6 is CYANIDE ION (CCD ID: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			2	1	1		
6	A	1	Total	C	N	0	0
			2	1	1		

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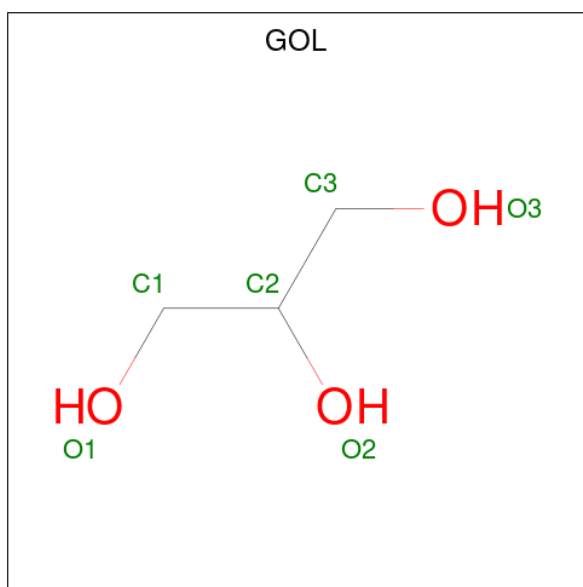
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			2	1	1		
6	C	1	Total	C	N	0	0
			2	1	1		

- Molecule 7 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	C	5	Total	O	0	0
			5	5		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

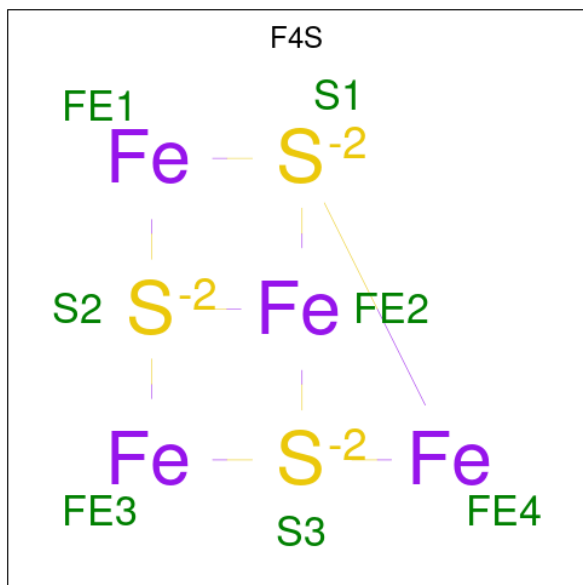


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

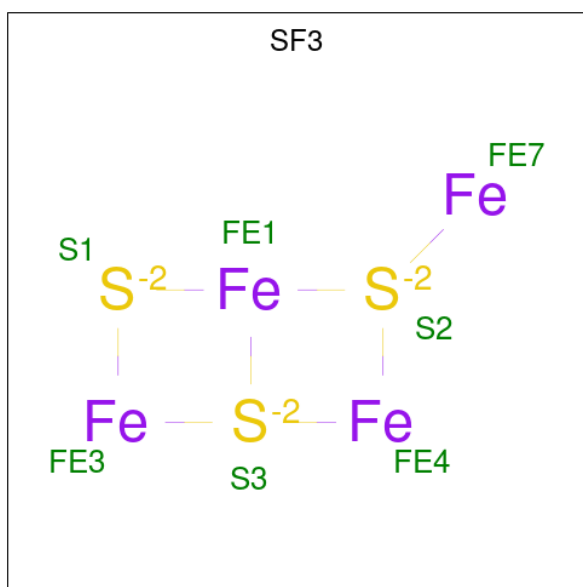
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	C	1	Total	Mg	0	0
			1	1		

- Molecule 10 is FE4-S3 CLUSTER (CCD ID: F4S) (formula: Fe_4S_3).



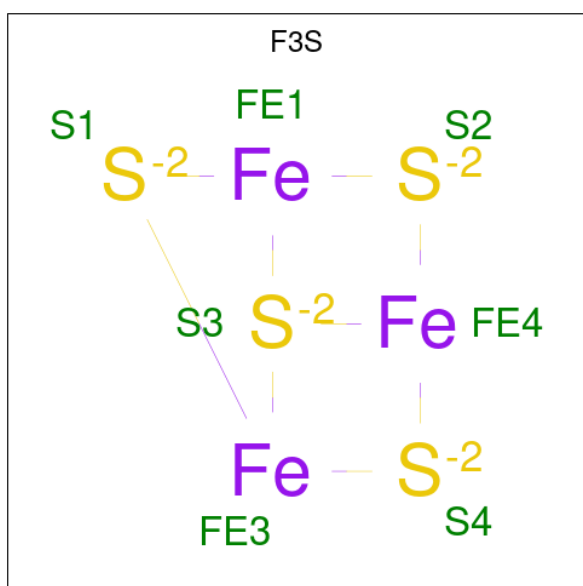
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	1
			7	4	3		
10	D	1	Total	Fe	S	0	1
			7	4	3		

- Molecule 11 is FE4-S3 CLUSTER (CCD ID: SF3) (formula: Fe_4S_3).



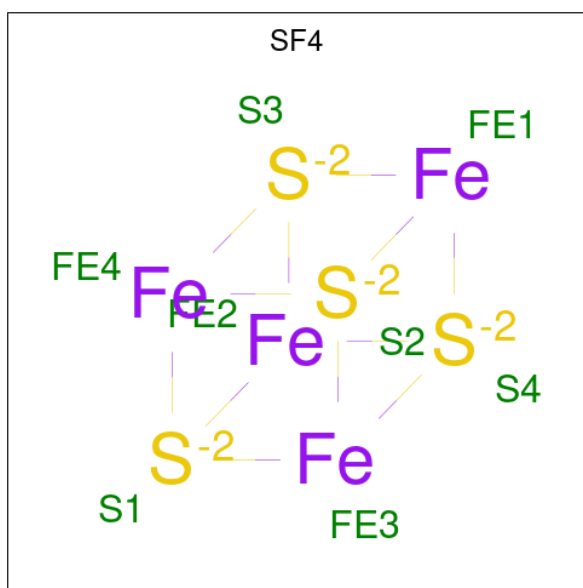
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	1
			7	4	3		
11	D	1	Total	Fe	S	0	1
			7	4	3		

- Molecule 12 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			7	3	4		
12	D	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	Fe	S	0	0
			8	4	4		
13	D	1	Total	Fe	S	0	0
			8	4	4		

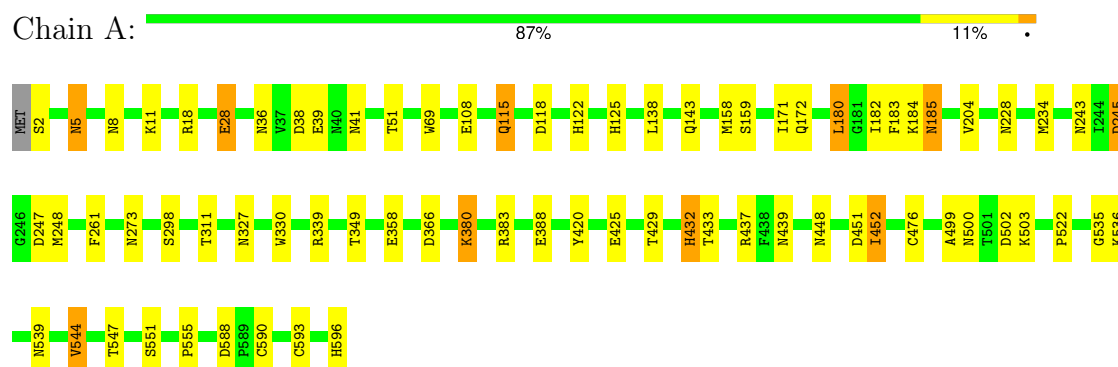
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	622	Total	O	0	0
			622	622		
14	B	253	Total	O	0	0
			253	253		
14	C	532	Total	O	0	0
			532	532		
14	D	224	Total	O	0	0
			224	224		

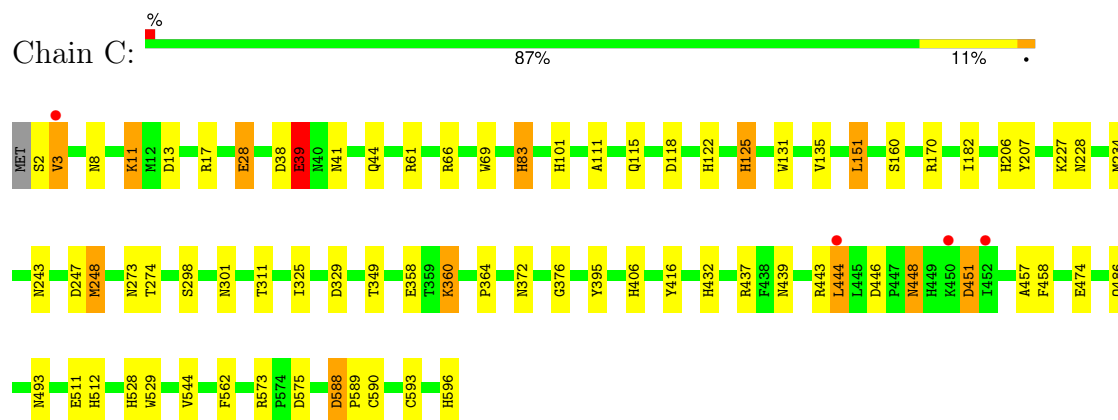
3 Residue-property plots

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.

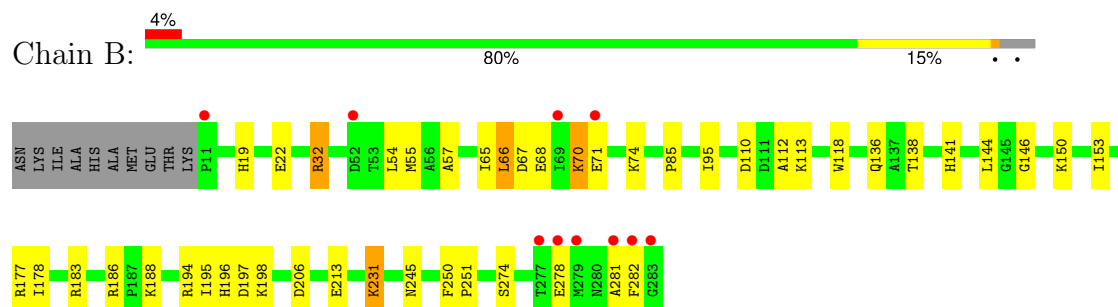
- Molecule 1: Membrane-bound hydrogenase large subunit



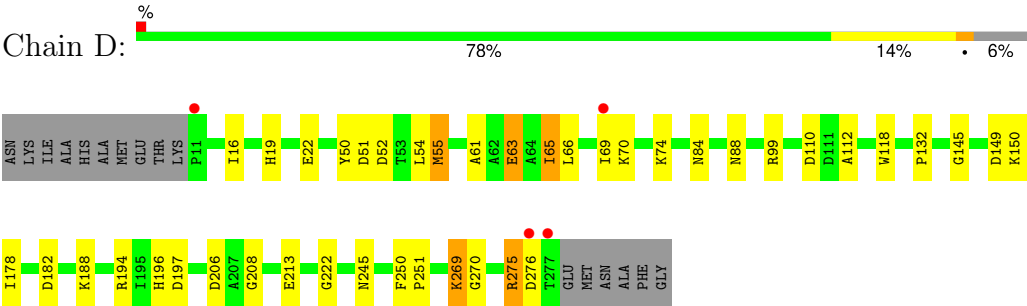
- Molecule 1: Membrane-bound hydrogenase large subunit



- Molecule 2: Membrane-bound hydrogenase small subunit



● Molecule 2: Membrane-bound hydrogenase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.65Å 116.66Å 113.61Å 90.00° 91.34° 90.00°	Depositor
Resolution (Å)	20.00 – 1.22 20.00 – 1.22	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.22) 91.0 (20.00-1.22)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.22Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.139 , 0.171 0.128 , 0.149	Depositor DCC
R_{free} test set	54353 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	10.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-l,-k 0.001 for -h,l,k 0.076 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15529	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: CYN, 3NI, FE2, F3S, SF4, O, CMO, F4S, GOL, MG, SF3

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	1.14	5/4952 (0.1%)	1.48	61/6739 (0.9%)
1	C	1.10	6/4919 (0.1%)	1.52	61/6698 (0.9%)
2	B	1.10	3/2241 (0.1%)	1.61	36/3032 (1.2%)
2	D	1.06	0/2190	1.59	42/2966 (1.4%)
All	All	1.11	14/14302 (0.1%)	1.53	200/19435 (1.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	ARG	CD-NE	8.70	1.58	1.46
1	A	588	ASP	C-O	-8.08	1.20	1.23
1	C	101	HIS	CB-CG	6.39	1.59	1.50
1	A	452	ILE	N-CA	-6.34	1.38	1.46
1	A	432	HIS	CG-ND1	-6.26	1.31	1.38
1	C	101	HIS	ND1-CE1	-6.02	1.26	1.32
2	B	194	ARG	CD-NE	-5.52	1.38	1.46
1	C	406	HIS	CE1-NE2	5.47	1.38	1.32
1	C	101	HIS	CG-CD2	5.44	1.41	1.35
1	A	383	ARG	CZ-NH1	5.39	1.40	1.32
2	B	141	HIS	ND1-CE1	-5.38	1.27	1.32
1	C	206	HIS	CE1-NE2	5.36	1.38	1.32
1	C	360	LYS	C-N	-5.36	1.30	1.33
2	B	250	PHE	CA-C	5.23	1.57	1.52

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	ASP	CA-CB-CG	13.57	126.17	112.60
2	D	275	ARG	CD-NE-CZ	12.40	141.77	124.40
1	A	500	ASN	CA-CB-CG	11.63	124.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	177	ARG	CG-CD-NE	-11.53	86.64	112.00
1	C	298	SER	CA-C-N	-11.23	104.65	122.73
1	C	298	SER	C-N-CA	-11.23	104.65	122.73
2	B	54	LEU	O-C-N	-11.04	109.12	122.48
1	C	41	ASN	CA-CB-CG	10.71	123.31	112.60
2	B	278	GLU	CA-C-O	10.51	133.19	120.57
2	D	110	ASP	CA-CB-CG	10.04	122.64	112.60
2	B	54	LEU	CA-C-O	10.04	129.71	118.97
2	B	177	ARG	CD-NE-CZ	9.93	138.31	124.40
1	A	596	HIS	CG-CD2-NE2	9.84	117.04	107.20
1	A	451	ASP	CA-C-N	9.67	134.13	120.98
1	A	451	ASP	C-N-CA	9.67	134.13	120.98
2	D	54	LEU	O-C-N	-9.16	111.64	122.27
1	A	432	HIS	CA-CB-CG	-9.15	104.65	113.80
1	C	69	TRP	CZ3-CH2-CZ2	9.03	133.24	121.50
1	A	311	THR	CA-C-O	-9.03	111.29	119.59
1	C	248	MET	CG-SD-CE	-8.95	81.20	100.90
2	D	70	LYS	CA-C-N	8.84	132.46	120.44
2	D	70	LYS	C-N-CA	8.84	132.46	120.44
1	A	248	MET	CG-SD-CE	-8.83	81.47	100.90
1	C	311	THR	CA-C-O	-8.71	111.57	119.59
1	C	448	ASN	CA-CB-CG	8.69	121.29	112.60
1	A	18	ARG	NE-CZ-NH2	8.62	126.96	119.20
1	C	311	THR	O-C-N	8.44	130.74	121.12
2	B	32	ARG	NE-CZ-NH2	8.31	126.68	119.20
1	C	28	GLU	CG-CD-OE1	8.27	137.41	118.40
1	C	125	HIS	CA-CB-CG	-8.24	105.56	113.80
1	A	448	ASN	CB-CG-ND2	-8.20	104.10	116.40
1	C	8	ASN	CA-CB-CG	8.19	120.79	112.60
1	A	8	ASN	CA-CB-CG	8.16	120.77	112.60
1	C	39	GLU	CB-CG-CD	8.10	126.37	112.60
1	A	502	ASP	CA-CB-CG	7.95	120.55	112.60
2	D	99	ARG	CD-NE-CZ	7.91	135.48	124.40
2	B	194	ARG	CD-NE-CZ	7.85	135.39	124.40
2	D	250	PHE	CA-CB-CG	7.84	121.64	113.80
1	A	69	TRP	CZ3-CH2-CZ2	7.77	131.60	121.50
1	C	458	PHE	CA-C-O	7.70	128.84	120.90
2	D	276	ASP	CA-C-O	7.68	129.49	120.58
1	A	125	HIS	CA-CB-CG	-7.65	106.15	113.80
1	C	122	HIS	CA-CB-CG	-7.62	106.18	113.80
1	A	41	ASN	OD1-CG-ND2	-7.49	115.11	122.60
2	D	197	ASP	CA-CB-CG	7.47	120.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	66	LEU	O-C-N	7.36	129.65	122.07
1	A	28	GLU	CG-CD-OE2	7.30	135.19	118.40
1	A	451	ASP	O-C-N	-7.22	113.99	122.87
2	B	196	HIS	CA-CB-CG	7.22	121.02	113.80
1	A	596	HIS	CE1-NE2-CD2	-7.15	101.85	109.00
2	D	196	HIS	CA-CB-CG	7.01	120.81	113.80
1	A	122	HIS	CA-CB-CG	-7.00	106.80	113.80
2	B	110	ASP	CA-CB-CG	6.92	119.52	112.60
2	D	269	LYS	O-C-N	-6.92	112.82	122.37
1	A	311	THR	O-C-N	6.88	128.96	121.12
1	C	451	ASP	CA-C-N	6.86	130.78	120.77
1	C	451	ASP	C-N-CA	6.86	130.78	120.77
2	B	67	ASP	CA-C-O	6.80	128.18	120.90
2	B	250	PHE	CA-CB-CG	6.80	120.60	113.80
1	A	28	GLU	CB-CG-CD	6.72	124.02	112.60
2	B	231	LYS	CG-CD-CE	6.72	126.76	111.30
1	C	432	HIS	CA-CB-CG	-6.72	107.08	113.80
2	B	146	GLY	O-C-N	6.68	130.22	122.68
2	B	66	LEU	O-C-N	6.67	128.94	122.07
2	D	194	ARG	NE-CZ-NH2	-6.62	113.24	119.20
1	C	273	ASN	CA-CB-CG	6.59	119.19	112.60
1	C	596	HIS	CG-CD2-NE2	6.58	113.78	107.20
2	B	186	ARG	NE-CZ-NH2	6.56	125.11	119.20
1	C	170	ARG	NE-CZ-NH2	-6.49	113.36	119.20
2	B	281	ALA	CA-C-O	-6.46	111.61	119.43
1	C	41	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	C	44	GLN	CG-CD-NE2	-6.44	106.74	116.40
2	B	274	SER	CA-C-N	6.43	130.00	120.87
2	B	274	SER	C-N-CA	6.43	130.00	120.87
1	C	358	GLU	CG-CD-OE2	-6.40	103.68	118.40
1	A	499	ALA	CA-C-N	6.39	132.00	123.05
1	A	499	ALA	C-N-CA	6.39	132.00	123.05
2	D	149	ASP	CA-CB-CG	6.39	118.99	112.60
2	D	55	MET	N-CA-C	6.38	120.29	110.20
2	D	213	GLU	CB-CG-CD	-6.38	101.76	112.60
1	C	416	TYR	CA-CB-CG	-6.37	102.43	113.90
1	A	298	SER	CA-C-N	6.32	129.92	120.31
1	A	298	SER	C-N-CA	6.32	129.92	120.31
1	C	13	ASP	CA-C-N	-6.32	113.11	122.83
1	C	13	ASP	C-N-CA	-6.32	113.11	122.83
2	B	55	MET	CA-C-N	6.29	128.61	120.44
2	B	55	MET	C-N-CA	6.29	128.61	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLU	CG-CD-OE1	-6.28	103.95	118.40
1	A	588	ASP	CA-CB-CG	6.28	118.88	112.60
2	D	276	ASP	CA-C-N	-6.26	110.43	121.70
2	D	276	ASP	C-N-CA	-6.26	110.43	121.70
2	B	55	MET	O-C-N	-6.25	115.64	123.01
1	A	273	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	588	ASP	CA-C-O	6.21	125.26	120.48
2	D	52[A]	ASP	O-C-N	-6.21	114.32	122.39
2	D	52[B]	ASP	O-C-N	-6.21	114.32	122.39
2	B	113	LYS	CA-C-O	6.16	127.08	120.24
2	D	177	ARG	CA-CB-CG	6.16	126.42	114.10
1	A	425	GLU	CB-CG-CD	6.13	123.02	112.60
2	B	282	PHE	O-C-N	6.09	130.14	122.22
2	D	194	ARG	NH1-CZ-NH2	6.06	127.17	119.30
2	D	145	GLY	CA-C-N	6.05	127.70	120.14
2	D	145	GLY	C-N-CA	6.05	127.70	120.14
1	A	18	ARG	NH1-CZ-NH2	-6.04	111.44	119.30
1	C	135	VAL	CA-C-O	6.03	127.24	120.85
1	C	439	ASN	CA-CB-CG	6.02	118.62	112.60
2	D	54	LEU	CA-C-O	5.99	125.49	118.90
2	D	269	LYS	CA-C-N	5.92	130.56	122.63
2	D	269	LYS	C-N-CA	5.92	130.56	122.63
1	A	36	ASN	CB-CG-ND2	-5.91	107.53	116.40
1	A	439	ASN	CA-CB-CG	5.89	118.49	112.60
1	C	125	HIS	CB-CG-CD2	-5.89	123.55	131.20
2	B	278	GLU	CB-CA-C	5.82	120.42	111.39
1	A	327	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	A	234	MET	CA-CB-CG	-5.79	102.51	114.10
2	D	51	ASP	CA-CB-CG	5.76	118.36	112.60
2	B	282	PHE	CB-CA-C	-5.75	101.70	111.02
1	A	39	GLU	CB-CG-CD	5.75	122.37	112.60
1	C	44	GLN	CG-CD-OE1	5.71	132.22	120.80
1	C	573	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	A	451	ASP	CA-C-O	5.66	127.42	121.19
1	C	3	VAL	O-C-N	5.66	129.06	123.18
1	A	5	ASN	OD1-CG-ND2	5.65	128.25	122.60
1	C	17	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	C	372	ASN	CA-CB-CG	5.63	118.23	112.60
1	C	395	TYR	CA-CB-CG	5.61	124.00	113.90
2	D	182	ASP	CA-CB-CG	5.60	118.20	112.60
2	D	55	MET	O-C-N	-5.59	116.41	123.01
2	B	278	GLU	O-C-N	-5.57	112.89	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	TRP	CE3-CZ3-CH2	-5.57	113.86	121.10
1	A	437	ARG	NE-CZ-NH1	-5.54	115.96	121.50
2	D	270	GLY	CA-C-O	5.52	126.40	122.37
1	A	448	ASN	CB-CG-OD1	5.52	131.84	120.80
1	A	358	GLU	CG-CD-OE2	-5.51	105.73	118.40
1	A	143	GLN	OE1-CD-NE2	5.50	128.10	122.60
1	C	38	ASP	CA-C-N	5.49	129.89	120.72
1	C	38	ASP	C-N-CA	5.49	129.89	120.72
1	C	69	TRP	CH2-CZ2-CE2	-5.46	110.40	117.50
1	A	118	ASP	CA-CB-CG	5.45	118.05	112.60
2	B	144	LEU	CA-C-N	5.45	129.34	121.44
2	B	144	LEU	C-N-CA	5.45	129.34	121.44
1	A	38	ASP	CA-CB-CG	5.34	117.94	112.60
2	D	118	TRP	CA-CB-CG	5.33	123.73	113.60
1	C	131	TRP	CA-C-N	5.33	130.12	123.14
1	C	131	TRP	C-N-CA	5.33	130.12	123.14
1	A	261	PHE	CA-CB-CG	5.32	119.12	113.80
2	B	65	ILE	CA-C-O	5.32	126.48	120.95
1	C	28	GLU	CG-CD-OE2	-5.31	106.20	118.40
1	C	437	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	183	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	383	ARG	CA-CB-CG	5.25	124.61	114.10
2	B	118	TRP	CA-CB-CG	5.25	123.56	113.60
1	C	376	GLY	O-C-N	-5.24	116.10	122.76
1	A	366	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	500	ASN	CB-CG-ND2	5.24	124.25	116.40
2	D	208	GLY	CA-C-N	5.22	130.11	122.85
2	D	208	GLY	C-N-CA	5.22	130.11	122.85
1	C	38	ASP	CA-C-O	5.22	127.78	121.88
2	B	282	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	108	GLU	CB-CG-CD	5.21	121.46	112.60
2	B	195	ILE	CA-CB-CG1	5.21	119.25	110.40
1	C	248	MET	CB-CG-SD	-5.20	97.10	112.70
1	C	83	HIS	CB-CG-CD2	-5.20	124.44	131.20
2	D	88	ASN	CA-CB-CG	5.19	117.79	112.60
1	C	486	GLN	OE1-CD-NE2	5.18	127.78	122.60
2	D	55	MET	CA-C-N	5.18	127.17	120.44
2	D	55	MET	C-N-CA	5.18	127.17	120.44
1	A	596	HIS	CB-CG-CD2	5.18	137.93	131.20
1	A	596	HIS	ND1-CG-CD2	-5.17	100.93	106.10
1	A	172	GLN	O-C-N	5.17	127.60	122.12
2	D	213	GLU	CG-CD-OE1	-5.17	106.52	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	275	ARG	N-CA-C	5.15	117.35	110.35
1	C	118	ASP	CA-CB-CG	5.14	117.74	112.60
2	B	278	GLU	N-CA-CB	-5.14	104.66	112.47
1	C	457	ALA	N-CA-CB	5.11	118.17	110.30
1	C	38	ASP	O-C-N	-5.11	115.44	122.23
1	A	383	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	D	275	ARG	CG-CD-NE	5.11	123.23	112.00
1	A	185	ASN	CA-C-N	-5.10	114.88	120.44
1	A	185	ASN	C-N-CA	-5.10	114.88	120.44
1	C	234	MET	CA-CB-CG	-5.09	103.92	114.10
1	A	245[A]	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	245[B]	ASP	CA-CB-CG	5.08	117.68	112.60
2	D	177	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	539	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	C	66	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	A	330	TRP	CD2-CE2-CZ2	5.06	127.46	122.40
1	C	588	ASP	CB-CA-C	5.05	115.39	111.00
1	A	339	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	C	125	HIS	CB-CG-ND1	5.04	130.26	122.70
1	C	562	PHE	CA-CB-CG	5.04	118.84	113.80
2	B	177	ARG	CB-CG-CD	-5.03	99.73	111.30
1	C	227	LYS	O-C-N	-5.03	118.48	123.46
1	C	83	HIS	CB-CG-ND1	5.03	130.24	122.70
1	A	185	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	C	575	ASP	CA-C-N	5.01	129.21	123.15
1	C	575	ASP	C-N-CA	5.01	129.21	123.15
1	C	329	ASP	CA-CB-CG	-5.01	107.59	112.60
2	B	213	GLU	CB-CG-CD	-5.00	104.09	112.60
2	D	84	ASN	N-CA-C	5.00	114.06	108.25

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	4770	0	4704	48	0
1	C	4750	0	4668	32	0
2	B	2159	0	2102	18	0
2	D	2109	0	2058	14	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
7	A	5	0	0	6	0
7	C	5	0	0	5	0
8	A	12	0	15	2	0
8	C	12	0	14	1	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	7	0	0	0	0
10	D	7	0	0	0	0
11	B	7	0	0	0	0
11	D	7	0	0	0	0
12	B	7	0	0	0	0
12	D	7	0	0	0	0
13	B	8	0	0	0	0
13	D	8	0	0	0	0
14	A	622	0	0	10	0
14	B	253	0	0	6	0
14	C	532	0	0	9	0
14	D	224	0	0	2	0
All	All	15529	0	13561	104	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 4.

All (104) 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:593:CYS:CB	7:C:607:O:O	2.13	0.95
1:A:593:CYS:CB	7:A:607:O:O	2.20	0.89
1:C:593:CYS:HB2	7:C:607:O:O	1.75	0.86
2:B:198[B]:LYS:HE3	14:B:1051:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HG	14:A:1377:HOH:O	1.82	0.79
1:A:184[A]:LYS:HD2	14:B:971:HOH:O	1.83	0.78
1:A:184[A]:LYS:HE3	14:A:914:HOH:O	1.83	0.77
1:A:593:CYS:HB2	7:A:607:O:O	1.86	0.75
1:C:274[A]:THR:HG22	1:C:474:GLU:OE2	1.87	0.74
14:A:1620:HOH:O	2:B:57:ALA:HA	1.88	0.73
1:A:5:ASN:HD21	1:A:11:LYS:NZ	1.88	0.71
2:B:112:ALA:O	2:B:150:LYS:HD2	1.95	0.67
1:C:151[A]:LEU:HD11	1:C:444:LEU:HD23	1.76	0.67
1:A:555:PRO:HA	14:A:1041:HOH:O	1.94	0.66
1:C:590:CYS:CB	7:C:606:O:O	2.43	0.66
1:C:593:CYS:N	7:C:607:O:O	2.30	0.65
1:C:444:LEU:HD13	14:C:1032:HOH:O	1.96	0.64
1:A:171[B]:ILE:HD11	1:A:204:VAL:HG11	1.78	0.64
1:A:593:CYS:N	7:A:607:O:O	2.31	0.63
1:A:535:GLY:O	1:A:536[B]:LYS:HE3	1.99	0.62
1:A:158[B]:MET:HE2	14:A:990:HOH:O	1.98	0.62
1:C:83:HIS:HD2	1:C:528:HIS:NE2	1.98	0.62
1:C:182:ILE:HG22	14:D:1308:HOH:O	1.99	0.61
1:A:5:ASN:HD21	1:A:11:LYS:HZ3	1.49	0.60
1:A:590:CYS:CB	7:A:606:O:O	2.49	0.60
1:A:115[B]:GLN:OE1	1:A:522:PRO:HG3	2.02	0.59
1:A:547:THR:O	1:A:551[B]:SER:HB3	2.01	0.59
1:C:349:THR:HB	14:C:1597:HOH:O	2.03	0.57
1:C:243:ASN:OD1	8:C:703:GOL:H31	2.04	0.57
1:A:228:ASN:HD21	2:B:32:ARG:HH21	1.53	0.57
1:A:349:THR:HG21	1:A:555:PRO:HG3	1.86	0.56
1:A:180:LEU:HD12	14:A:959:HOH:O	2.05	0.56
1:C:446:ASP:OD1	1:C:448:ASN:HB2	2.07	0.55
1:C:228:ASN:H	2:D:245:ASN:HD21	1.55	0.54
1:C:28:GLU:OE2	7:C:608:O:O	2.25	0.54
1:C:111:ALA:O	1:C:115[B]:GLN:HG2	2.07	0.54
1:C:39:GLU:H	1:C:39:GLU:CD	2.16	0.53
2:B:206:ASP:OD2	2:D:206:ASP:OD2	2.27	0.52
2:D:172:MET:HE3	2:D:178[A]:ILE:HD13	1.91	0.52
2:B:183[A]:ARG:HG3	14:B:1223:HOH:O	2.09	0.51
2:D:61:ALA:O	2:D:65[A]:ILE:HD12	2.10	0.51
1:A:184[B]:LYS:HG3	1:A:185:ASN:N	2.25	0.51
1:A:228:ASN:H	2:B:245:ASN:HD21	1.59	0.51
1:A:544[B]:VAL:HG11	1:A:593:CYS:HB3	1.92	0.51
2:D:63:GLU:HG2	14:D:1273:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:HIS:HE1	1:C:593:CYS:SG	2.35	0.50
2:D:16:ILE:HD11	2:D:69:ILE:HG21	1.94	0.49
1:A:243:ASN:OD1	8:A:703:GOL:H31	2.13	0.49
1:A:182:ILE:HG22	14:B:584:HOH:O	2.12	0.48
1:C:247[B]:ASP:OD1	1:C:248:MET:HG2	2.14	0.48
1:A:544[A]:VAL:HG21	1:A:593:CYS:HB3	1.95	0.48
1:A:247[B]:ASP:OD2	2:D:188:LYS:HD3	2.14	0.47
1:C:3:VAL:CG1	1:C:11:LYS:HG3	2.45	0.47
1:A:536[B]:LYS:HE3	14:A:767:HOH:O	2.15	0.47
2:B:198[A]:LYS:CE	14:C:1560:HOH:O	2.63	0.47
2:B:198[A]:LYS:HE3	14:C:1560:HOH:O	2.14	0.47
2:D:19:HIS:HD1	2:D:22[A]:GLU:CD	2.23	0.46
8:A:703:GOL:H12	14:A:1319:HOH:O	2.15	0.46
1:A:536[B]:LYS:HD2	14:A:962:HOH:O	2.15	0.46
2:D:50:TYR:CD1	2:D:55:MET:HE1	2.51	0.46
1:A:184[A]:LYS:HE2	2:B:68:GLU:OE1	2.15	0.46
2:B:188:LYS:NZ	14:C:1400:HOH:O	2.49	0.46
1:C:61[B]:ARG:NH2	14:C:764:HOH:O	2.49	0.46
1:C:151[A]:LEU:CD1	1:C:444:LEU:HD23	2.45	0.46
2:B:19:HIS:HD1	2:B:22[B]:GLU:CD	2.23	0.46
1:C:443:ARG:NH1	1:C:451:ASP:OD1	2.48	0.46
1:A:28:GLU:OE1	7:A:608:O:O	2.34	0.46
2:B:136[A]:GLN:NE2	14:B:293:HOH:O	2.49	0.45
1:A:245[A]:ASP:OD1	2:D:177:ARG:NH1	2.47	0.45
1:C:443:ARG:NH2	1:C:451:ASP:OD1	2.50	0.45
2:D:112:ALA:O	2:D:150:LYS:HD2	2.16	0.45
1:A:5:ASN:ND2	1:A:11:LYS:NZ	2.61	0.45
1:C:511:GLU:HG2	1:C:512:HIS:CD2	2.52	0.44
1:A:2:SER:N	14:A:908:HOH:O	2.49	0.44
2:B:70:LYS:NZ	14:B:1093:HOH:O	2.51	0.44
1:A:380:LYS:NZ	1:A:388:GLU:OE1	2.50	0.44
1:A:171[B]:ILE:CD1	1:A:204:VAL:HG11	2.46	0.44
1:C:2:SER:N	14:C:1592:HOH:O	2.50	0.44
2:B:70:LYS:O	2:B:70:LYS:HG3	2.11	0.44
1:A:5:ASN:HD21	1:A:11:LYS:CE	2.30	0.43
14:C:1560:HOH:O	2:D:222:GLY:HA3	2.18	0.43
1:C:125:HIS:HE1	1:C:207:TYR:O	2.00	0.43
1:A:349:THR:CG2	1:A:555:PRO:HG3	2.48	0.43
1:C:588:ASP:N	1:C:589:PRO:HD3	2.34	0.43
1:A:544[B]:VAL:CG1	1:A:593:CYS:HB3	2.49	0.43
1:A:138:LEU:HD21	1:A:171[B]:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:PRO:HG2	2:D:178[B]:ILE:CD1	2.49	0.43
1:C:364:PRO:HB2	1:C:529:TRP:CD2	2.54	0.42
1:A:452:ILE:HA	1:A:452:ILE:HD13	1.77	0.42
1:C:544[B]:VAL:HG21	1:C:593:CYS:HB3	2.01	0.42
1:A:429:THR:O	1:A:433[A]:THR:HG23	2.20	0.42
1:C:301:ASN:HA	1:C:325:ILE:O	2.20	0.41
1:A:51:THR:HB	2:B:95:ILE:HB	2.02	0.41
2:B:153:ILE:HD11	2:B:178[A]:ILE:HD12	2.02	0.41
1:A:115[B]:GLN:HG3	1:A:476:CYS:SG	2.61	0.41
1:A:115[A]:GLN:NE2	1:A:522:PRO:HA	2.35	0.41
1:A:159:SER:HG	1:C:160[B]:SER:HB3	1.86	0.41
1:A:420:TYR:OH	1:A:432:HIS:HE1	2.04	0.41
2:B:85:PRO:HD2	2:B:138:THR:O	2.21	0.40
1:A:544[A]:VAL:HG22	1:A:547:THR:OG1	2.21	0.40
1:A:593:CYS:CA	7:A:607:O:O	2.68	0.40
1:C:493:ASN:HB2	14:C:1409:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	612/596 (103%)	599 (98%)	13 (2%)	0	100	100
1	C	608/596 (102%)	595 (98%)	13 (2%)	0	100	100
2	B	279/283 (99%)	269 (96%)	10 (4%)	0	100	100
2	D	273/283 (96%)	262 (96%)	11 (4%)	0	100	100
All	All	1772/1758 (101%)	1725 (97%)	47 (3%)	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	523/505 (104%)	516 (99%)	7 (1%)	61	25
1	C	519/505 (103%)	513 (99%)	6 (1%)	63	28
2	B	233/233 (100%)	227 (97%)	6 (3%)	40	7
2	D	229/233 (98%)	221 (96%)	8 (4%)	32	3
All	All	1504/1476 (102%)	1477 (98%)	27 (2%)	55	16

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115[A]	GLN
1	A	115[B]	GLN
1	A	180	LEU
1	A	380	LYS
1	A	503	LYS
1	A	544[A]	VAL
1	A	544[B]	VAL
2	B	66	LEU
2	B	70	LYS
2	B	71	GLU
2	B	74	LYS
2	B	231	LYS
2	B	251	PRO
1	C	11	LYS
1	C	39	GLU
1	C	151[A]	LEU
1	C	151[B]	LEU
1	C	360	LYS
1	C	444	LEU
2	D	63	GLU
2	D	65[A]	ILE
2	D	65[B]	ILE
2	D	74	LYS
2	D	132	PRO

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Mol	Chain	Res	Type
2	D	251	PRO
2	D	269	LYS
2	D	275	ARG

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

Mol	Chain	Res	Type
1	A	5	ASN
1	A	36	ASN
1	A	41	ASN
1	A	136	ASN
1	A	168	GLN
1	A	172	GLN
1	A	185	ASN
1	A	228	ASN
1	A	268	GLN
1	A	273	ASN
1	A	327	ASN
1	A	430	GLN
1	A	432	HIS
1	A	439	ASN
1	A	486	GLN
1	A	493	ASN
2	B	104	GLN
2	B	245	ASN
1	C	41	ASN
1	C	83	HIS
1	C	125	HIS
1	C	168	GLN
1	C	232	ASN
1	C	273	ASN
1	C	430	GLN
1	C	432	HIS
1	C	439	ASN
1	C	486	GLN
1	C	493	ASN
2	D	193	GLN
2	D	245	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 ⓘ

Of 34 ligands modelled in this entry, 16 are monoatomic - leaving 18 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	$\# Z > 2$
12	F3S	D	308	2	0,9,9	-	-	-		
5	CMO	C	603	-	0,1,1	-	-	-		
10	F4S	D	301[A]	2	0,9,9	-	-	-		
13	SF4	B	309	2	0,12,12	-	-	-		
11	SF3	D	302[B]	2	0,8,8	-	-	-		
5	CMO	A	603	-	0,1,1	-	-	-		
6	CYN	A	605	-	1,1,1	0.28	0	-		
6	CYN	C	604	-	1,1,1	0.28	0	-		
8	GOL	C	703	-	5,5,5	1.35	0	5,5,5	2.53	2 (40%)
11	SF3	B	302[B]	2	0,8,8	-	-	-		
6	CYN	A	604	-	1,1,1	0.13	0	-		
13	SF4	D	309	2	0,12,12	-	-	-		
12	F3S	B	308	2	0,9,9	-	-	-		
8	GOL	C	702	-	5,5,5	0.69	0	5,5,5	3.81	3 (60%)
10	F4S	B	301[A]	2	0,9,9	-	-	-		
6	CYN	C	605	-	1,1,1	0.26	0	-		
8	GOL	A	703	-	5,5,5	0.90	0	5,5,5	4.45	5 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	702	-	5,5,5	0.97	0	5,5,5	1.98	3 (60%)

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
12	F3S	D	308	2	-	-	0/3/3/3
10	F4S	D	301[A]	2	-	-	0/4/3/3
13	SF4	B	309	2	-	-	0/6/5/5
11	SF3	D	302[B]	2	-	-	0/2/2/2
8	GOL	C	703	-	-	3/4/4/4	-
11	SF3	B	302[B]	2	-	-	0/2/2/2
13	SF4	D	309	2	-	-	0/6/5/5
12	F3S	B	308	2	-	-	0/3/3/3
8	GOL	C	702	-	-	1/4/4/4	-
10	F4S	B	301[A]	2	-	-	0/4/3/3
8	GOL	A	703	-	-	0/4/4/4	-
8	GOL	A	702	-	-	0/4/4/4	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	702	GOL	C3-C2-C1	-7.04	85.97	111.80
8	A	703	GOL	C3-C2-C1	-5.92	90.09	111.80
8	A	703	GOL	O2-C2-C3	4.91	129.50	109.18
8	A	703	GOL	O2-C2-C1	4.40	127.38	109.18
8	C	703	GOL	O2-C2-C1	4.39	127.35	109.18
8	A	703	GOL	O3-C3-C2	-3.62	94.06	110.38
8	C	703	GOL	O2-C2-C3	3.31	122.87	109.18
8	C	702	GOL	O3-C3-C2	-3.13	96.31	110.38
8	C	702	GOL	O2-C2-C3	-3.05	96.54	109.18
8	A	702	GOL	O2-C2-C1	2.87	121.06	109.18
8	A	703	GOL	O1-C1-C2	2.69	122.48	110.38
8	A	702	GOL	O1-C1-C2	2.16	120.08	110.38
8	A	702	GOL	O3-C3-C2	-2.02	101.29	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	702	GOL	O1-C1-C2-C3
8	C	703	GOL	C1-C2-C3-O3
8	C	703	GOL	O1-C1-C2-O2
8	C	703	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	703	GOL	1	0
8	A	703	GOL	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	595/596 (99%)	-0.57	0 100 100	4, 10, 26, 58	19 (3%)
1	C	595/596 (99%)	-0.40	4 (0%) 84 87	5, 13, 33, 63	15 (2%)
2	B	273/283 (96%)	-0.48	10 (3%) 45 46	4, 9, 32, 59	8 (2%)
2	D	267/283 (94%)	-0.42	4 (1%) 72 73	5, 11, 33, 64	8 (2%)
All	All	1730/1758 (98%)	-0.47	18 (1%) 79 81	4, 11, 31, 64	50 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	277	THR	4.2
2	B	281	ALA	3.8
2	B	282	PHE	3.7
2	B	283	GLY	3.3
2	B	11	PRO	3.0
2	D	11	PRO	2.8
2	D	276	ASP	2.7
2	D	69	ILE	2.6
2	B	278	GLU	2.6
2	B	279	MET	2.5
1	C	444	LEU	2.4
1	C	3	VAL	2.3
1	C	450	LYS	2.3
2	B	277	THR	2.3
2	B	69	ILE	2.2
2	B	52	ASP	2.2
1	C	452	ILE	2.1
2	B	71	GLU	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
7	O	C	607	1/1	0.91	0.07	8,8,8,8	1
8	GOL	C	702	6/6	0.91	0.10	21,23,30,43	0
7	O	A	607	1/1	0.92	0.08	8,8,8,8	1
8	GOL	C	703	6/6	0.93	0.09	18,25,29,34	0
7	O	C	609	1/1	0.94	0.11	8,8,8,8	1
7	O	C	606	1/1	0.94	0.10	14,14,14,14	0
7	O	C	608	1/1	0.94	0.07	9,9,9,9	1
7	O	A	606	1/1	0.95	0.08	12,12,12,12	0
8	GOL	A	702	6/6	0.95	0.07	19,22,26,29	0
7	O	A	609	1/1	0.96	0.16	7,7,7,7	1
8	GOL	A	703	6/6	0.96	0.07	18,28,34,35	0
7	O	A	608	1/1	0.97	0.12	9,9,9,9	1
7	O	C	610	1/1	0.97	0.10	7,7,7,7	1
7	O	A	610	1/1	0.98	0.17	8,8,8,8	1
5	CMO	C	603	2/2	0.99	0.04	8,8,8,10	0
6	CYN	A	604	2/2	0.99	0.03	6,6,6,7	0
6	CYN	A	605	2/2	0.99	0.03	6,6,6,6	0
6	CYN	C	605	2/2	0.99	0.03	8,8,8,8	0
4	3NI	A	602	1/1	0.99	0.07	12,12,12,12	0
5	CMO	A	603	2/2	0.99	0.02	6,6,6,7	0
6	CYN	C	604	2/2	1.00	0.04	9,9,9,9	0
3	FE2	A	601	1/1	1.00	0.01	6,6,6,6	0
4	3NI	C	602	1/1	1.00	0.08	15,15,15,15	0
3	FE2	C	601	1/1	1.00	0.01	8,8,8,8	0
9	MG	A	701	1/1	1.00	0.01	6,6,6,6	0
9	MG	C	701	1/1	1.00	0.01	8,8,8,8	0
10	F4S	B	301[A]	7/7	1.00	0.01	6,6,7,7	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	F4S	D	301[A]	7/7	1.00	0.01	7,8,9,9	7
11	SF3	B	302[B]	7/7	1.00	0.01	6,6,7,10	7
11	SF3	D	302[B]	7/7	1.00	0.02	7,8,9,11	7
12	F3S	B	308	7/7	1.00	0.01	5,5,5,6	0
12	F3S	D	308	7/7	1.00	0.01	6,6,7,7	0
13	SF4	B	309	8/8	1.00	0.01	6,6,7,7	0
13	SF4	D	309	8/8	1.00	0.01	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.