



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:42 AM UTC

PDB ID : 3AYX / pdb_00003ayx
Title : Membrane-bound respiratory [NiFe] hydrogenase from *Hydrogenovibrio marinus* in an H₂-reduced condition
Authors : Shomura, Y.; Yoon, K.S.; Nishihara, H.; Higuchi, Y.
Deposited on : 2011-05-20
Resolution : 1.18 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

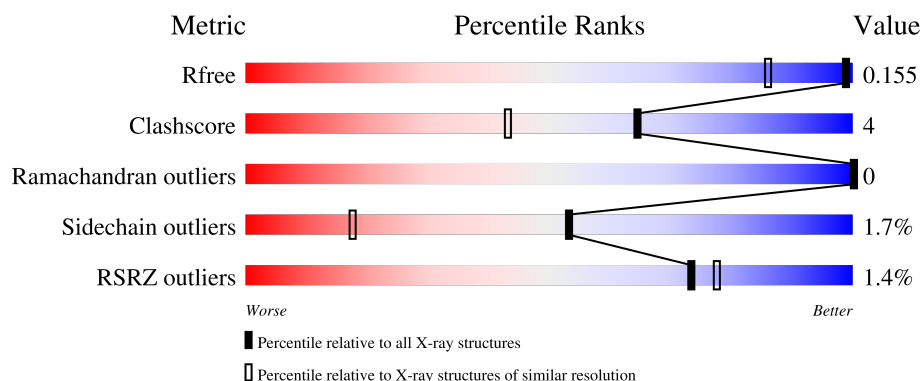
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.18 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	1789 (1.20-1.16)
Clashscore	190562	1845 (1.20-1.16)
Ramachandran outliers	187476	1789 (1.20-1.16)
Sidechain outliers	187428	1789 (1.20-1.16)
RSRZ outliers	180081	1787 (1.20-1.16)

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	0% 89% 9% .
1	C	596	0% 86% 12% .
2	B	283	2% 83% 12% ..
2	D	283	2% 79% 13% 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	606	-	-	X	-
7	O	C	607	-	-	X	-
8	GOL	A	703	-	-	X	-
8	GOL	C	703	-	X	-	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 15472 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	14	0
			4739	3008	825	880	26			
1	C	595	Total	C	N	O	S	0	14	0
			4739	3010	827	877	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	7	0
			2151	1366	366	398	21			
2	D	267	Total	C	N	O	S	0	5	0
			2092	1328	356	387	21			

- 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 (II) ION (CCD ID: NI) (formula: Ni).

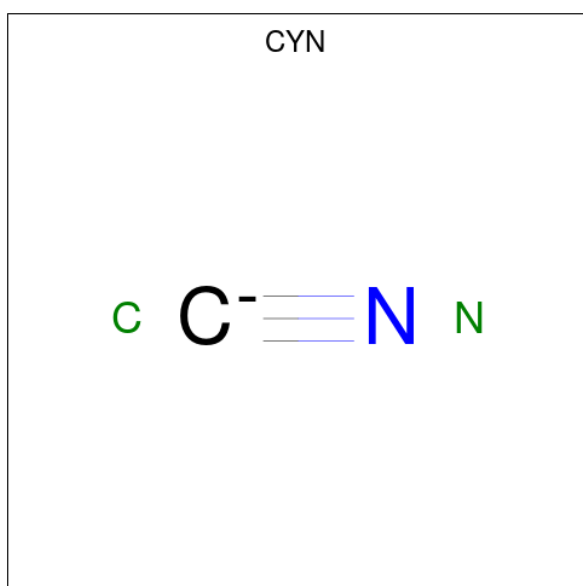
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		

- 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		

Continued on next page...

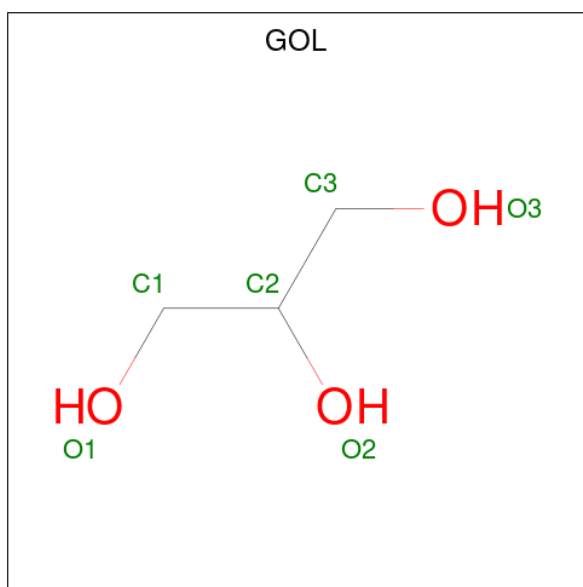
Continued from previous page...

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).

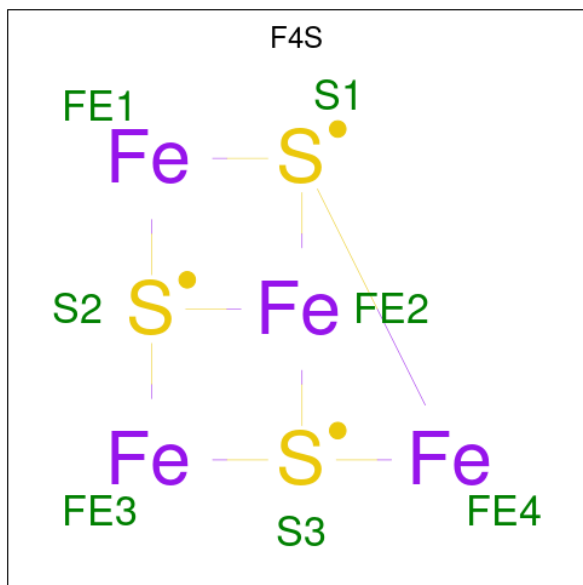


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

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

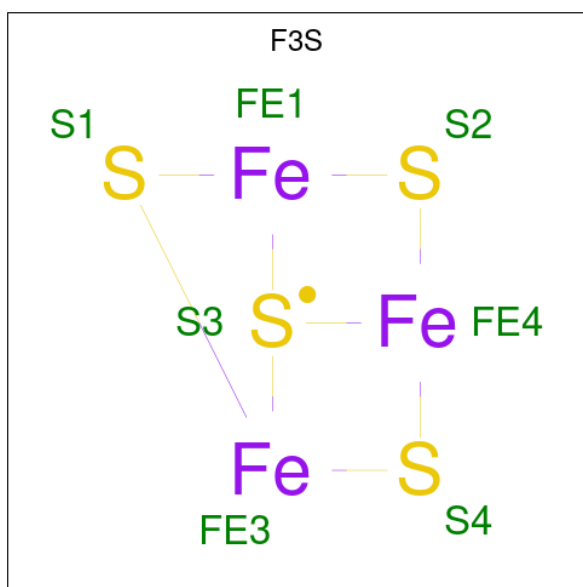
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	C	1	Total	Mg	0	0
			1	1		

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



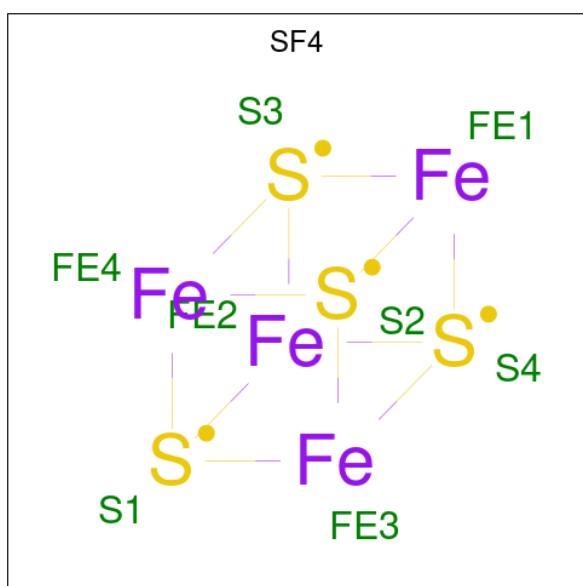
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	4	3		
10	D	1	Total	Fe	S	0	0
			7	4	3		

- Molecule 11 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

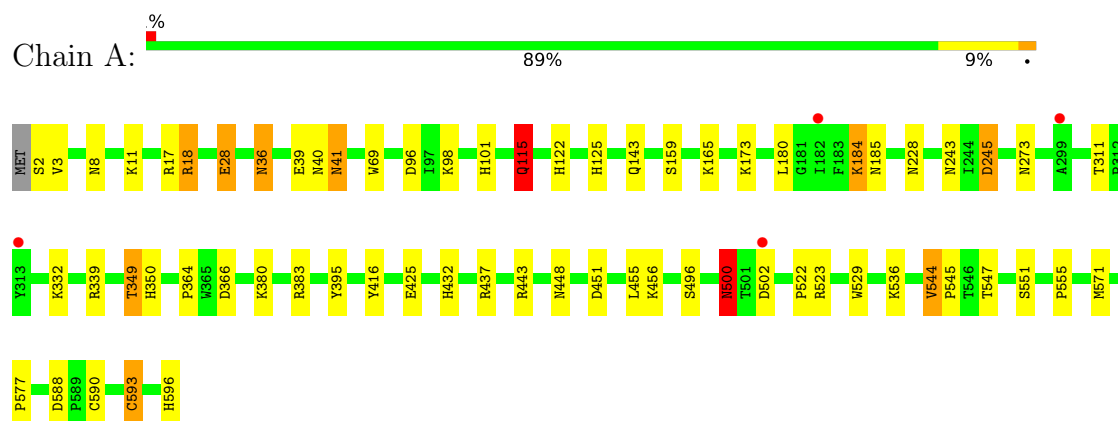
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	638	Total 638	O 638	0	0
13	B	271	Total 271	O 271	0	0
13	C	529	Total 529	O 529	0	0
13	D	217	Total 217	O 217	0	0

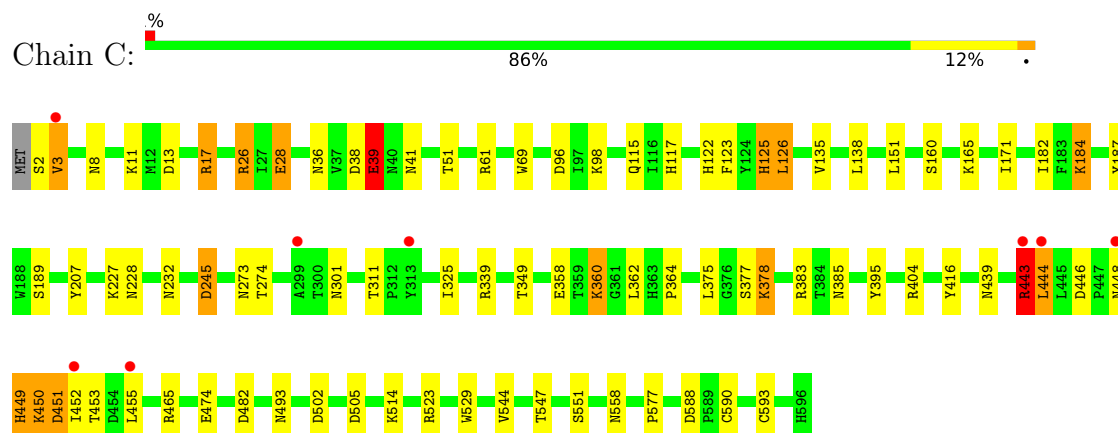
3 Residue-property plots [i](#)

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.

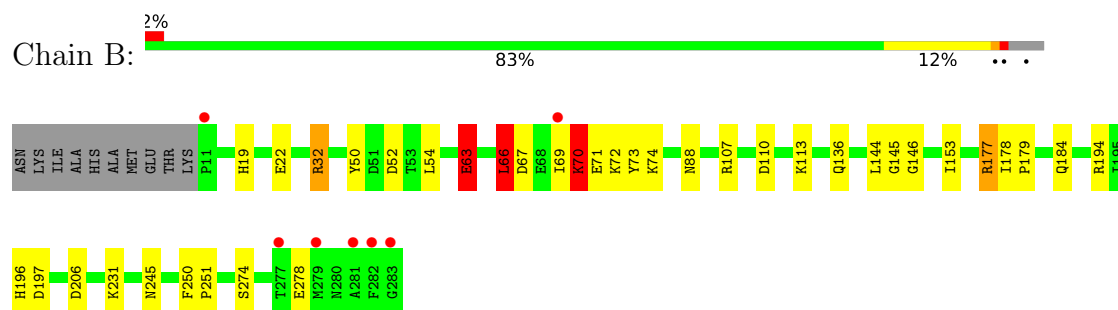
- Molecule 1: Membrane-bound hydrogenase large subunit



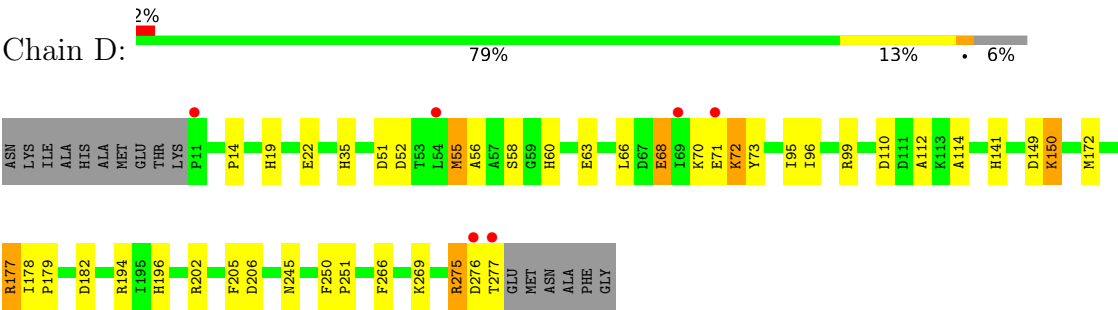
- Molecule 1: Membrane-bound hydrogenase large subunit



- 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	75.73Å 116.33Å 113.63Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	20.00 – 1.18 20.00 – 1.18	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.18) 89.6 (20.00-1.18)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.18Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.139 , 0.169 0.133 , 0.155	Depositor DCC
R_{free} test set	59041 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-l,-k 0.003 for -h,l,k 0.095 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15472	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: NI, F3S, SF4, GOL, F4S, CYN, CMO, O, MG, FE2

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	1.19	5/4905 (0.1%)	1.51	49/6679 (0.7%)
1	C	1.16	3/4909 (0.1%)	1.63	70/6685 (1.0%)
2	B	1.15	1/2230 (0.0%)	1.57	33/3019 (1.1%)
2	D	1.16	0/2164	1.63	37/2931 (1.3%)
All	All	1.17	9/14208 (0.1%)	1.58	189/19314 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	HIS	CB-CG	8.74	1.62	1.50
1	C	360	LYS	C-N	-8.43	1.27	1.33
1	A	588	ASP	C-O	-7.72	1.20	1.23
1	A	101	HIS	CG-CD2	6.10	1.42	1.35
1	C	449	HIS	CE1-NE2	-6.08	1.26	1.32
1	C	449	HIS	ND1-CE1	-5.58	1.26	1.32
1	A	18	ARG	CZ-NH2	-5.44	1.26	1.33
1	A	383	ARG	NE-CZ	-5.33	1.27	1.33
2	B	177	ARG	CZ-NH2	5.18	1.40	1.33

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	449	HIS	ND1-CE1-NE2	23.02	131.41	108.40
1	C	17	ARG	CD-NE-CZ	16.88	148.03	124.40
1	A	500	ASN	CA-CB-CG	16.45	129.05	112.60
1	C	449	HIS	CE1-NE2-CD2	-14.78	94.22	109.00
1	C	443	ARG	CD-NE-CZ	11.99	141.19	124.40
1	C	383	ARG	NE-CZ-NH1	11.68	133.18	121.50
2	B	177	ARG	CD-NE-CZ	11.42	140.39	124.40
1	A	245[A]	ASP	CA-CB-CG	11.03	123.63	112.60
1	A	245[B]	ASP	CA-CB-CG	11.03	123.63	112.60
1	A	502	ASP	CA-CB-CG	10.98	123.58	112.60
1	A	383	ARG	NE-CZ-NH1	-10.81	110.69	121.50
1	C	493	ASN	OD1-CG-ND2	-10.73	111.87	122.60
2	D	52	ASP	CA-CB-CG	-10.18	102.42	112.60
1	C	69	TRP	CZ3-CH2-CZ2	10.00	134.50	121.50
1	A	18	ARG	NE-CZ-NH2	9.88	128.09	119.20
1	C	502	ASP	CA-CB-CG	9.68	122.28	112.60
1	C	311	THR	CA-C-O	-9.62	111.28	119.36
2	D	70	LYS	CA-C-N	9.48	133.97	120.79
2	D	70	LYS	C-N-CA	9.48	133.97	120.79
1	C	135	VAL	CA-C-O	9.46	130.88	120.85
1	A	41	ASN	OD1-CG-ND2	-9.37	113.23	122.60
1	A	500	ASN	OD1-CG-ND2	-9.34	113.26	122.60
2	B	278	GLU	CA-C-O	9.22	132.25	121.28
1	A	432	HIS	CA-CB-CG	-9.20	104.60	113.80
1	C	558	ASN	OD1-CG-ND2	9.11	131.71	122.60
2	D	68	GLU	CA-CB-CG	8.96	132.01	114.10
2	D	275	ARG	NE-CZ-NH2	8.67	127.00	119.20
1	C	115	GLN	OE1-CD-NE2	-8.56	114.03	122.60
1	C	41	ASN	CA-CB-CG	8.55	121.15	112.60
1	A	451	ASP	CA-C-N	8.51	131.95	120.63
1	A	451	ASP	C-N-CA	8.51	131.95	120.63
1	C	449	HIS	CG-ND1-CE1	-8.50	94.85	109.30
1	A	39	GLU	CB-CG-CD	8.44	126.95	112.60
2	D	275	ARG	O-C-N	8.36	132.72	122.86
1	A	448	ASN	CB-CG-ND2	-8.35	103.88	116.40
1	C	39	GLU	CB-CG-CD	8.24	126.61	112.60
1	C	451	ASP	CA-C-N	8.24	133.45	122.90
1	C	451	ASP	C-N-CA	8.24	133.45	122.90
1	A	122	HIS	CA-CB-CG	-8.21	105.59	113.80
2	B	274	SER	CA-C-N	8.11	132.38	120.87
2	B	274	SER	C-N-CA	8.11	132.38	120.87
2	B	110	ASP	CA-CB-CG	8.09	120.69	112.60
1	A	339	ARG	NE-CZ-NH2	-7.86	112.13	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	ARG	NE-CZ-NH2	7.76	126.19	119.20
1	A	380	LYS	CA-CB-CG	7.62	129.34	114.10
2	B	145	GLY	CA-C-N	7.60	129.63	120.14
2	B	145	GLY	C-N-CA	7.60	129.63	120.14
1	A	332	LYS	CB-CG-CD	7.55	128.67	111.30
1	A	115	GLN	OE1-CD-NE2	-7.55	115.05	122.60
1	A	28	GLU	CG-CD-OE2	7.52	135.70	118.40
1	C	69	TRP	CE3-CZ3-CH2	-7.52	111.33	121.10
2	D	177	ARG	NE-CZ-NH1	7.41	128.91	121.50
2	D	177	ARG	NE-CZ-NH2	-7.41	112.53	119.20
2	D	276	ASP	CA-C-N	-7.40	108.37	121.70
2	D	276	ASP	C-N-CA	-7.40	108.37	121.70
2	B	196	HIS	CA-CB-CG	7.40	121.20	113.80
1	C	8	ASN	CA-CB-CG	7.35	119.95	112.60
2	B	146	GLY	O-C-N	7.31	129.98	122.24
2	D	250	PHE	CA-CB-CG	7.29	121.09	113.80
2	B	274	SER	O-C-N	-7.27	114.28	122.86
2	B	70	LYS	CA-C-N	7.22	130.45	120.63
2	B	70	LYS	C-N-CA	7.22	130.45	120.63
1	A	437	ARG	NH1-CZ-NH2	7.20	128.66	119.30
2	B	250	PHE	CA-CB-CG	7.18	120.98	113.80
2	D	58	SER	CA-C-O	7.10	129.73	121.49
1	C	135	VAL	O-C-N	-7.07	114.55	121.83
1	A	69	TRP	CZ3-CH2-CZ2	7.07	130.69	121.50
1	A	596	HIS	CG-CD2-NE2	7.01	114.21	107.20
1	C	28	GLU	CG-CD-OE1	6.98	134.46	118.40
1	A	437	ARG	NE-CZ-NH1	-6.96	114.53	121.50
2	D	149	ASP	CA-CB-CG	6.95	119.55	112.60
2	D	66	LEU	O-C-N	6.92	129.20	122.07
1	A	184	LYS	CA-CB-CG	6.91	127.91	114.10
1	A	596	HIS	CE1-NE2-CD2	-6.75	102.25	109.00
1	C	358	GLU	CG-CD-OE2	-6.72	102.95	118.40
1	C	273	ASN	CA-CB-CG	6.70	119.30	112.60
1	A	448	ASN	OD1-CG-ND2	6.58	129.18	122.60
2	D	177	ARG	CA-CB-CG	-6.57	100.96	114.10
1	C	416	TYR	CA-CB-CG	-6.55	102.10	113.90
2	B	194	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	C	395	TYR	CA-CB-CG	6.46	125.53	113.90
2	B	184	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	C	453	THR	CA-C-N	6.42	133.62	122.32
1	C	453	THR	C-N-CA	6.42	133.62	122.32
2	B	197	ASP	CA-CB-CG	6.39	118.99	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	ASP	CA-C-O	6.37	125.39	120.48
2	D	51	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	273	ASN	CA-CB-CG	6.33	118.94	112.60
1	C	439	ASN	CA-CB-CG	6.23	118.83	112.60
1	C	125	HIS	CA-CB-CG	-6.23	107.57	113.80
1	C	122	HIS	CA-CB-CG	-6.20	107.60	113.80
2	D	110	ASP	CA-CB-CG	6.17	118.78	112.60
2	D	14	PRO	O-C-N	6.17	130.01	123.10
1	A	36	ASN	CB-CG-ND2	-6.16	107.16	116.40
1	A	18	ARG	NH1-CZ-NH2	-6.09	111.38	119.30
2	B	144	LEU	CA-C-N	6.09	130.27	121.44
2	B	144	LEU	C-N-CA	6.09	130.27	121.44
2	D	71	GLU	O-C-N	-6.07	115.58	122.08
2	D	196	HIS	CA-CB-CG	6.05	119.85	113.80
1	C	452	ILE	CA-C-O	-6.04	114.01	120.59
2	D	63	GLU	CA-C-O	6.03	126.94	120.55
1	A	588	ASP	CA-CB-CG	6.02	118.62	112.60
2	B	113	LYS	CA-C-O	5.99	126.77	120.42
1	C	588	ASP	CB-CA-C	5.97	116.20	111.00
1	A	8	ASN	CA-CB-CG	5.96	118.56	112.60
2	B	67	ASP	CA-C-O	5.95	127.06	120.82
2	B	107	ARG	CA-CB-CG	5.92	125.94	114.10
2	B	107	ARG	NE-CZ-NH2	-5.91	113.88	119.20
1	A	383	ARG	NH1-CZ-NH2	5.91	126.98	119.30
2	B	66[A]	LEU	O-C-N	5.90	128.37	122.12
2	B	66[B]	LEU	O-C-N	5.90	128.37	122.12
1	A	500	ASN	CB-CG-OD1	5.89	132.57	120.80
1	A	311	THR	O-C-N	5.87	128.57	121.29
1	A	173	LYS	CA-CB-CG	5.84	125.78	114.10
1	A	17	ARG	NE-CZ-NH2	-5.78	114.00	119.20
2	D	141	HIS	ND1-CE1-NE2	5.75	114.15	108.40
2	B	194	ARG	NH1-CZ-NH2	5.72	126.73	119.30
1	C	383	ARG	NH1-CZ-NH2	-5.71	111.87	119.30
1	C	558	ASN	CB-CG-ND2	-5.67	107.89	116.40
2	D	275	ARG	CA-C-O	-5.67	115.38	121.56
1	A	383	ARG	CD-NE-CZ	5.67	132.34	124.40
1	C	36	ASN	CA-C-O	-5.67	114.58	120.70
1	C	123	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	125	HIS	CA-CB-CG	-5.65	108.15	113.80
1	A	593	CYS	CB-CA-C	-5.65	102.01	110.88
1	C	451	ASP	CA-C-O	5.61	127.67	121.56
2	D	56	ALA	CA-C-O	5.60	126.47	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	378	LYS	CA-C-O	5.60	126.11	119.56
1	C	117	HIS	CA-CB-CG	-5.59	108.21	113.80
1	C	227	LYS	O-C-N	-5.59	117.93	123.46
1	A	96	ASP	CB-CG-OD1	5.58	131.23	118.40
1	C	451	ASP	CB-CG-OD2	-5.58	105.58	118.40
2	B	54	LEU	CA-C-O	5.55	124.91	118.97
2	D	35	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
2	D	194	ARG	NH1-CZ-NH2	5.54	126.50	119.30
1	C	245[A]	ASP	CA-CB-CG	-5.54	107.06	112.60
1	C	245[B]	ASP	CA-CB-CG	-5.54	107.06	112.60
2	D	269	LYS	CA-C-N	5.52	130.97	122.85
2	D	269	LYS	C-N-CA	5.52	130.97	122.85
2	B	278	GLU	O-C-N	-5.50	115.04	122.41
1	C	404	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	443	ARG	NE-CZ-NH1	-5.49	116.01	121.50
2	D	182	ASP	CA-CB-CG	5.45	118.05	112.60
1	C	385	ASN	CA-CB-CG	-5.45	107.15	112.60
1	C	3	VAL	O-C-N	5.45	128.31	123.03
1	A	425	GLU	CB-CG-CD	5.42	121.82	112.60
1	C	13	ASP	CA-C-N	-5.42	114.57	122.86
1	C	13	ASP	C-N-CA	-5.42	114.57	122.86
1	C	69	TRP	CH2-CZ2-CE2	-5.41	110.47	117.50
1	A	416	TYR	CA-CB-CG	-5.38	104.22	113.90
1	C	451	ASP	O-C-N	-5.37	116.52	122.86
1	C	452	ILE	N-CA-C	-5.36	100.16	107.99
1	C	125	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	A	28	GLU	CB-CG-CD	5.34	121.69	112.60
1	C	184	LYS	CA-C-N	5.32	130.11	122.40
1	C	184	LYS	C-N-CA	5.32	130.11	122.40
2	D	277	THR	N-CA-CB	-5.31	102.47	111.50
2	B	88	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	C	38	ASP	CA-C-N	5.31	129.09	120.60
1	C	38	ASP	C-N-CA	5.31	129.09	120.60
2	D	55	MET	N-CA-C	5.29	118.32	110.48
2	D	266	PHE	CA-CB-CG	5.29	119.09	113.80
1	C	482	ASP	CA-CB-CG	5.29	117.89	112.60
2	D	99	ARG	CD-NE-CZ	5.29	131.80	124.40
1	C	505	ASP	CB-CG-OD1	5.28	130.53	118.40
1	A	366	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	8	ASN	O-C-N	-5.27	115.00	122.06
1	C	189	SER	CA-C-O	5.26	125.65	119.28
2	D	114	ALA	CA-C-O	-5.26	115.61	121.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	231	LYS	CG-CD-CE	5.25	123.38	111.30
2	B	63[A]	GLU	CA-C-O	5.23	126.01	120.10
2	B	63[B]	GLU	CA-C-O	5.23	126.01	120.10
1	C	377[A]	SER	N-CA-C	-5.22	106.89	113.20
1	C	377[B]	SER	N-CA-C	-5.22	106.89	113.20
2	B	69	ILE	O-C-N	5.16	127.14	121.83
1	A	395	TYR	CA-CB-CG	5.15	123.17	113.90
1	C	3	VAL	N-CA-CB	5.14	118.68	112.10
1	C	450	LYS	CA-C-N	-5.12	112.91	120.94
1	C	450	LYS	C-N-CA	-5.12	112.91	120.94
1	C	375	LEU	CA-C-N	5.09	124.93	120.10
1	C	375	LEU	C-N-CA	5.09	124.93	120.10
1	C	26	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
1	C	465	ARG	NE-CZ-NH1	5.08	126.58	121.50
2	D	205	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	383	ARG	CA-CB-CG	5.08	124.26	114.10
1	C	232	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	41	ASN	CB-CG-ND2	5.03	123.94	116.40
2	B	54	LEU	O-C-N	-5.02	116.41	122.48
2	D	60	HIS	CE1-NE2-CD2	-5.02	103.98	109.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	ARG	Sidechain

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	4739	0	4657	38	0
1	C	4739	0	4663	50	0
2	B	2151	0	2091	13	0
2	D	2092	0	2032	12	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
6	C	4	0	0	0	0
7	A	5	0	0	4	0
7	C	5	0	0	6	0
8	A	12	0	15	4	0
8	C	12	0	15	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	8	0	0	0	0
12	D	8	0	0	0	0
13	A	638	0	0	9	0
13	B	271	0	0	3	0
13	C	529	0	0	13	0
13	D	217	0	0	3	0
All	All	15472	0	13473	107	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 (107) 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:590:CYS:CB	7:A:606:O:O	2.09	0.99
1:C:590:CYS:CB	7:C:606:O:O	2.08	0.97
1:C:151[A]:LEU:HD11	1:C:444:LEU:HD23	1.64	0.78
1:C:274[A]:THR:HG22	1:C:474:GLU:OE2	1.86	0.75
8:A:703:GOL:H32	13:A:1420:HOH:O	1.88	0.74
2:B:136:GLN:HG2	13:B:1448:HOH:O	1.88	0.73
1:A:544[B]:VAL:HG11	1:A:593:CYS:HB3	1.77	0.67
1:A:349[A]:THR:HB	13:A:1347:HOH:O	1.95	0.66
1:A:544[A]:VAL:HG21	1:A:593:CYS:HB3	1.78	0.66
1:A:547:THR:O	1:A:551[B]:SER:HB3	1.96	0.64
1:C:593:CYS:N	7:C:607:O:O	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:CYS:N	7:A:607:O:O	2.29	0.63
1:C:138:LEU:HD21	1:C:171[A]:ILE:HG22	1.81	0.63
1:C:593:CYS:CB	7:C:607:O:O	2.49	0.61
1:C:544[A]:VAL:HG11	1:C:593:CYS:HB3	1.83	0.61
1:A:593:CYS:CB	7:A:607:O:O	2.48	0.61
1:A:228:ASN:HD21	2:B:32:ARG:HH21	1.49	0.61
1:C:349:THR:HB	13:C:1385:HOH:O	2.00	0.61
2:B:72:LYS:HG2	2:B:73:TYR:CE2	2.35	0.60
1:C:544[B]:VAL:HG11	1:C:593:CYS:HB3	1.86	0.58
1:A:3:VAL:HG11	1:A:11:LYS:HE2	1.85	0.58
1:C:444:LEU:HD13	13:C:1576:HOH:O	2.04	0.57
1:A:571:MET:HE1	1:A:577:PRO:HB3	1.87	0.57
1:A:184:LYS:HE2	13:A:1043:HOH:O	2.05	0.56
1:C:544[A]:VAL:CG1	1:C:593:CYS:HB3	2.36	0.55
2:B:63[A]:GLU:HG2	13:B:350:HOH:O	2.07	0.55
2:B:206:ASP:OD2	2:D:206:ASP:OD2	2.24	0.55
1:C:449:HIS:HD2	13:C:1327:HOH:O	1.90	0.55
1:A:544[B]:VAL:CG1	1:A:593:CYS:HB3	2.37	0.54
1:C:228:ASN:H	2:D:245:ASN:HD21	1.56	0.54
2:D:68:GLU:O	2:D:72:LYS:HB2	2.07	0.54
1:A:228:ASN:H	2:B:245:ASN:HD21	1.57	0.53
1:C:26:ARG:O	1:C:126[B]:LEU:HD13	2.07	0.53
1:C:28:GLU:OE2	7:C:608:O:O	2.27	0.53
2:D:72:LYS:HE2	2:D:73:TYR:CZ	2.45	0.52
2:D:172[B]:MET:HG2	2:D:177:ARG:O	2.09	0.52
1:C:182:ILE:HG22	13:D:1323:HOH:O	2.11	0.51
1:A:571:MET:HE1	1:A:577:PRO:CB	2.42	0.50
1:A:243:ASN:OD1	8:A:703:GOL:H12	2.11	0.50
1:C:590:CYS:HB2	7:C:606:O:O	1.96	0.50
1:A:245[A]:ASP:OD1	8:A:703:GOL:O1	2.31	0.48
1:C:138:LEU:HD21	1:C:171[A]:ILE:CG2	2.42	0.48
1:C:39:GLU:H	1:C:39:GLU:CD	2.22	0.48
1:C:182:ILE:HG23	13:C:920:HOH:O	2.12	0.48
2:D:72:LYS:HE2	2:D:73:TYR:CE2	2.49	0.48
1:A:523:ARG:CD	1:A:590:CYS:HB2	2.43	0.48
2:B:177:ARG:NH1	1:C:245[B]:ASP:OD2	2.47	0.47
1:C:61[B]:ARG:NH2	13:C:1247:HOH:O	2.47	0.47
1:C:378:LYS:HE2	13:C:928:HOH:O	2.12	0.47
2:D:19:HIS:HD1	2:D:22[B]:GLU:CD	2.21	0.47
1:A:143[B]:GLN:HG2	13:A:1437:HOH:O	2.14	0.47
2:D:55:MET:HE3	13:D:1199:HOH:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASP:OD1	1:C:98:LYS:NZ	2.48	0.47
1:C:523:ARG:CD	1:C:590:CYS:HB2	2.45	0.46
1:C:61[A]:ARG:NH1	13:C:1633:HOH:O	2.49	0.46
1:C:125:HIS:HE1	1:C:207:TYR:O	1.97	0.46
1:A:456:LYS:HD3	13:A:1487:HOH:O	2.16	0.45
1:C:61[B]:ARG:NH2	13:C:780:HOH:O	2.46	0.45
1:C:360:LYS:HE2	1:C:362:LEU:HD23	1.97	0.45
1:A:40:ASN:O	1:A:41:ASN:HB2	2.16	0.45
1:A:28:GLU:OE1	7:A:608:O:O	2.35	0.45
1:A:2:SER:N	13:A:1548:HOH:O	2.49	0.45
2:B:72:LYS:HG2	2:B:73:TYR:CD2	2.51	0.45
1:A:165:LYS:HE3	13:A:888:HOH:O	2.17	0.45
1:C:245[A]:ASP:OD1	8:C:703:GOL:O1	2.34	0.45
2:B:50:TYR:CD1	2:B:66[A]:LEU:HD13	2.52	0.44
1:C:339:ARG:HD3	13:C:689:HOH:O	2.17	0.44
1:C:544[B]:VAL:HG12	1:C:547:THR:H	1.82	0.44
1:A:349[B]:THR:OG1	1:A:555:PRO:HG3	2.18	0.44
1:A:544[B]:VAL:HG12	1:A:545:PRO:HD2	2.00	0.44
1:C:593:CYS:HB2	7:C:607:O:O	2.16	0.44
2:D:55:MET:HB2	13:D:1199:HOH:O	2.18	0.44
2:D:112:ALA:O	2:D:150:LYS:HE3	2.17	0.43
2:B:19:HIS:HD1	2:B:22[B]:GLU:CD	2.25	0.43
1:C:151[A]:LEU:HD21	1:C:444:LEU:HD21	2.00	0.43
1:A:159:SER:HG	1:C:160[B]:SER:HB3	1.84	0.43
1:C:2:SER:N	13:C:1026:HOH:O	2.50	0.43
1:C:26:ARG:HA	1:C:126[B]:LEU:HD22	2.00	0.43
1:C:51:THR:HB	2:D:95:ILE:HB	1.99	0.43
1:C:443:ARG:NH2	1:C:451:ASP:OD1	2.48	0.43
1:A:115:GLN:NE2	1:A:522:PRO:HA	2.33	0.43
1:A:536:LYS:NZ	13:A:825:HOH:O	2.49	0.43
1:A:364:PRO:HB2	1:A:529:TRP:CD2	2.53	0.43
1:A:455:LEU:HA	1:A:455:LEU:HD23	1.83	0.42
1:C:26:ARG:CA	1:C:126[B]:LEU:HD22	2.49	0.42
1:C:446:ASP:OD1	1:C:448:ASN:HB2	2.19	0.42
1:A:571:MET:HB3	1:A:571:MET:HE2	1.89	0.42
1:C:547:THR:O	1:C:551[B]:SER:HB3	2.20	0.42
1:A:500:ASN:C	1:A:500:ASN:HD22	2.28	0.42
1:A:496:SER:CB	8:A:703:GOL:H31	2.50	0.42
1:C:3:VAL:HG13	1:C:11:LYS:HG3	2.02	0.42
1:A:593:CYS:CB	6:A:605:CYN:C	2.98	0.42
1:C:544[B]:VAL:HG11	1:C:593:CYS:C	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349[A]:THR:HG22	1:A:350:HIS:CD2	2.55	0.41
1:C:184:LYS:NZ	13:C:1322:HOH:O	2.53	0.41
1:C:165:LYS:HD3	13:C:1196:HOH:O	2.20	0.41
2:B:153:ILE:HD11	2:B:178[B]:ILE:HG23	2.02	0.41
2:B:70:LYS:NZ	13:B:895:HOH:O	2.49	0.41
1:A:544[A]:VAL:HG22	1:A:547:THR:OG1	2.20	0.41
1:C:364:PRO:HB2	1:C:529:TRP:CD2	2.56	0.41
1:C:514:LYS:NZ	13:C:1462:HOH:O	2.53	0.41
1:C:301:ASN:HA	1:C:325:ILE:O	2.21	0.41
1:A:185:ASN:ND2	13:A:1090:HOH:O	2.54	0.41
1:A:18:ARG:HH21	1:A:36:ASN:HD21	1.68	0.40
2:B:178[B]:ILE:HG23	2:B:179:PRO:HD2	2.03	0.40
2:D:178[B]:ILE:HG23	2:D:179:PRO:HD2	2.02	0.40
1:C:187:TYR:CE2	1:C:577:PRO:HD2	2.57	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	607/596 (102%)	596 (98%)	11 (2%)	0	100	100
1	C	607/596 (102%)	597 (98%)	10 (2%)	0	100	100
2	B	278/283 (98%)	269 (97%)	9 (3%)	0	100	100
2	D	270/283 (95%)	259 (96%)	11 (4%)	0	100	100
All	All	1762/1758 (100%)	1721 (98%)	41 (2%)	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	518/505 (103%)	510 (98%)	8 (2%)	57	21
1	C	518/505 (103%)	510 (98%)	8 (2%)	57	21
2	B	232/233 (100%)	223 (96%)	9 (4%)	28	3
2	D	226/233 (97%)	221 (98%)	5 (2%)	45	10
All	All	1494/1476 (101%)	1464 (98%)	30 (2%)	53	12

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LYS
1	A	115	GLN
1	A	180	LEU
1	A	349[A]	THR
1	A	349[B]	THR
1	A	500	ASN
1	A	544[A]	VAL
1	A	544[B]	VAL
2	B	52	ASP
2	B	63[A]	GLU
2	B	63[B]	GLU
2	B	66[A]	LEU
2	B	66[B]	LEU
2	B	70	LYS
2	B	71	GLU
2	B	74	LYS
2	B	251	PRO
1	C	17	ARG
1	C	39	GLU
1	C	126[A]	LEU
1	C	126[B]	LEU
1	C	443	ARG
1	C	444	LEU
1	C	450	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	455	LEU
2	D	72	LYS
2	D	96	ILE
2	D	150	LYS
2	D	251	PRO
2	D	275	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	115	GLN
1	A	172	GLN
1	A	185	ASN
1	A	228	ASN
1	A	232	ASN
1	A	273	ASN
1	A	327	ASN
1	A	372	ASN
1	A	430	GLN
1	A	432	HIS
1	A	439	ASN
1	A	486	GLN
1	A	493	ASN
1	A	500	ASN
2	B	245	ASN
1	C	5	ASN
1	C	41	ASN
1	C	125	HIS
1	C	168	GLN
1	C	172	GLN
1	C	232	ASN
1	C	273	ASN
1	C	327	ASN
1	C	430	GLN
1	C	432	HIS
1	C	439	ASN
1	C	449	HIS
1	C	486	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 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	CYN	A	605	-	1,1,1	0.38	0	-		
12	SF4	D	309	2	0,12,12	-	-	-		
8	GOL	C	702	-	5,5,5	0.60	0	5,5,5	1.64	1 (20%)
5	CMO	C	603	-	0,1,1	-	-	-		
6	CYN	A	604	-	1,1,1	0.28	0	-		
6	CYN	C	604	-	1,1,1	0.27	0	-		
10	F4S	D	301	2	0,9,9	-	-	-		
5	CMO	A	603	-	0,1,1	-	-	-		
8	GOL	A	702	-	5,5,5	0.87	0	5,5,5	2.11	1 (20%)
8	GOL	A	703	-	5,5,5	1.01	0	5,5,5	3.14	2 (40%)
8	GOL	C	703	-	5,5,5	1.36	1 (20%)	5,5,5	5.53	4 (80%)
11	F3S	B	308	2	0,9,9	-	-	-		
11	F3S	D	308	2	0,9,9	-	-	-		
6	CYN	C	605	-	1,1,1	0.19	0	-		
10	F4S	B	301	2	0,9,9	-	-	-		
12	SF4	B	309	2	0,12,12	-	-	-		

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	703	GOL	C1-C2	2.01	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	703	GOL	O2-C2-C3	7.11	138.61	109.18
8	C	703	GOL	C3-C2-C1	-6.81	86.82	111.80
8	A	703	GOL	O2-C2-C1	5.89	133.57	109.18
8	C	703	GOL	O1-C1-C2	-5.45	85.86	110.38
8	C	703	GOL	O2-C2-C1	5.13	130.41	109.18
8	A	702	GOL	O1-C1-C2	-3.49	94.65	110.38
8	A	703	GOL	O1-C1-C2	-3.49	94.67	110.38
8	C	702	GOL	C3-C2-C1	-3.04	100.66	111.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	605	CYN	1	0
8	A	703	GOL	4	0
8	C	703	GOL	1	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%)	-0.30	4 (0%) 84 89	5, 12, 27, 49	14 (2%)
1	C	595/596 (99%)	-0.12	8 (1%) 75 79	7, 14, 34, 61	14 (2%)
2	B	273/283 (96%)	-0.23	7 (2%) 57 59	7, 11, 32, 53	7 (2%)
2	D	267/283 (94%)	-0.12	6 (2%) 62 65	7, 13, 39, 71	5 (1%)
All	All	1730/1758 (98%)	-0.20	25 (1%) 73 77	5, 13, 32, 71	40 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	277	THR	5.9
1	C	444	LEU	3.6
2	B	11	PRO	3.2
2	D	276	ASP	3.2
2	B	277	THR	3.0
2	D	11	PRO	2.9
2	B	281	ALA	2.9
2	D	69	ILE	2.7
2	B	282	PHE	2.6
1	C	443	ARG	2.5
2	B	69	ILE	2.5
1	C	299	ALA	2.5
1	A	182	ILE	2.4
1	C	313	TYR	2.4
1	C	455	LEU	2.3
1	A	299	ALA	2.2
2	B	283	GLY	2.2
1	A	502	ASP	2.1
1	C	452	ILE	2.1
1	C	3	VAL	2.1
2	D	71	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	313	TYR	2.0
1	C	448	ASN	2.0
2	B	279	MET	2.0
2	D	54	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	O	A	607	1/1	0.86	0.09	8,8,8,8	1
7	O	A	606	1/1	0.91	0.13	11,11,11,11	1
7	O	C	607	1/1	0.91	0.07	9,9,9,9	1
7	O	C	609	1/1	0.92	0.07	8,8,8,8	1
8	GOL	C	702	6/6	0.92	0.09	23,26,30,39	0
8	GOL	C	703	6/6	0.94	0.09	19,28,33,39	0
8	GOL	A	703	6/6	0.95	0.09	19,32,37,42	0
7	O	A	608	1/1	0.95	0.12	12,12,12,12	1
8	GOL	A	702	6/6	0.95	0.08	21,24,27,41	0
7	O	A	609	1/1	0.96	0.27	7,7,7,7	1
7	O	C	608	1/1	0.96	0.08	11,11,11,11	1
7	O	A	610	1/1	0.96	0.21	8,8,8,8	1
7	O	C	610	1/1	0.96	0.11	8,8,8,8	1
7	O	C	606	1/1	0.98	0.10	11,11,11,11	1
6	CYN	C	605	2/2	0.98	0.04	9,9,9,10	0
5	CMO	A	603	2/2	0.98	0.04	7,7,7,10	0
6	CYN	C	604	2/2	0.99	0.03	9,9,9,11	0
5	CMO	C	603	2/2	0.99	0.03	10,10,10,11	0
6	CYN	A	604	2/2	0.99	0.03	7,7,7,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CYN	A	605	2/2	0.99	0.04	8,8,8,9	0
3	FE2	A	601	1/1	1.00	0.02	8,8,8,8	0
3	FE2	C	601	1/1	1.00	0.01	10,10,10,10	0
4	NI	A	602	1/1	1.00	0.09	12,12,12,12	0
4	NI	C	602	1/1	1.00	0.09	14,14,14,14	0
9	MG	A	701	1/1	1.00	0.01	7,7,7,7	0
9	MG	C	701	1/1	1.00	0.01	10,10,10,10	0
10	F4S	B	301	7/7	1.00	0.01	7,7,8,8	0
10	F4S	D	301	7/7	1.00	0.02	9,9,9,9	0
11	F3S	B	308	7/7	1.00	0.01	7,7,7,7	0
11	F3S	D	308	7/7	1.00	0.02	8,8,8,8	0
12	SF4	B	309	8/8	1.00	0.01	8,8,8,8	0
12	SF4	D	309	8/8	1.00	0.01	8,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.