



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:36 AM EDT

PDB ID : 1QH8 / pdb_00001qh8
Title : NITROGENASE MOFE PROTEIN FROM KLEBSIELLA PNEUMONIAE,
AS-CRYSTALLIZED (MIXED OXIDATION) STATE
Authors : Mayer, S.M.; Lawson, D.M.; Gormal, C.A.; Roe, S.M.; Smith, B.E.
Deposited on : 1999-05-11
Resolution : 1.60 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

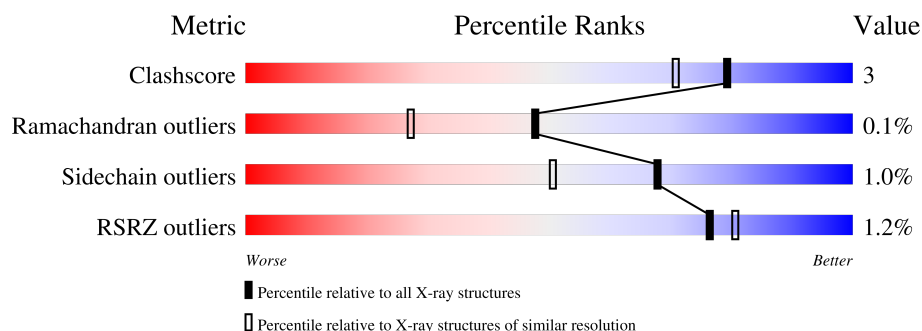
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	478	87% 12%
1	C	478	86% 13%
2	B	519	90% 10%
2	D	519	91% 9%

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	EDO	B	2907	-	X	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18565 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 PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	4	0
			3709	2360	633	692	24			
1	C	478	Total	C	N	O	S	0	2	0
			3716	2368	635	689	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	VAL	ALA	conflict	UNP P00466
A	94	GLY	GLU	conflict	UNP P09772
C	85	VAL	ALA	conflict	UNP P00466
C	94	GLY	GLU	conflict	UNP P09772

- Molecule 2 is a protein called PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	519	Total	C	N	O	S	0	6	0
			4067	2598	681	760	28			
2	D	519	Total	C	N	O	S	0	6	0
			4060	2590	679	762	29			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

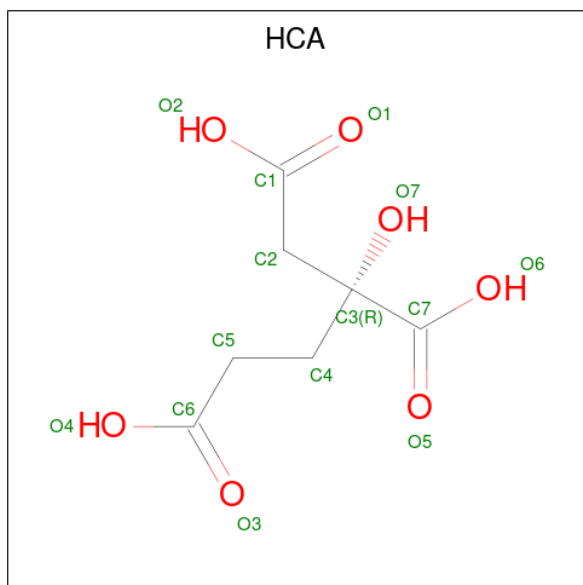
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	3	Total	Mg	0	0
			3	3		
3	C	1	Total	Mg	0	0
			1	1		

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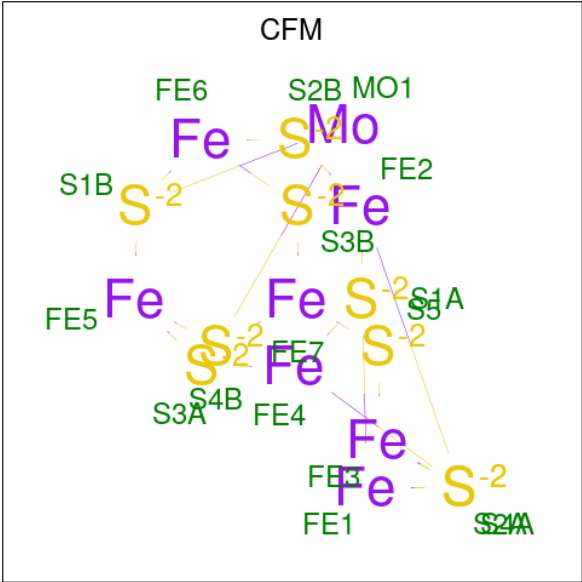
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



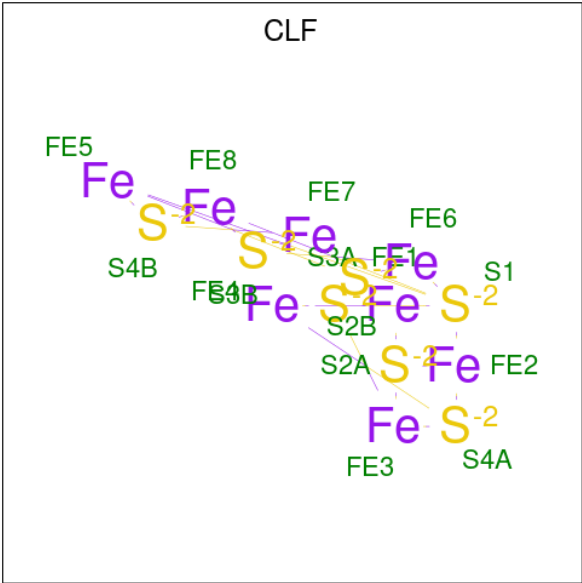
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe_7MoS_9).



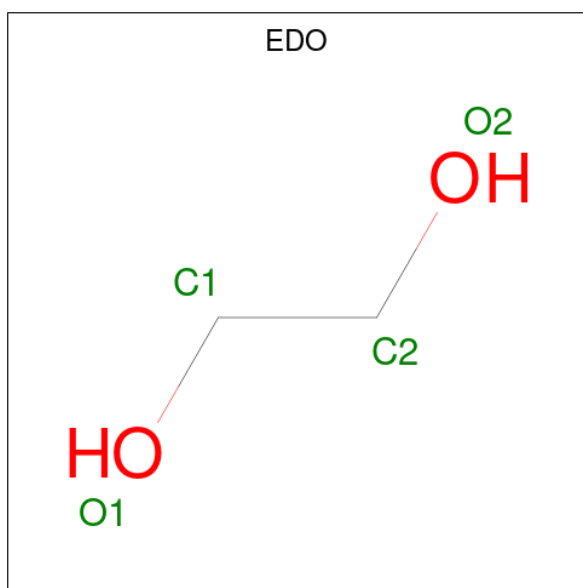
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	1
			17	10	7		
6	C	1	Total	Fe	S	0	1
			17	10	7		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cl 1 1	0	0
8	D	1	Total Cl 1 1	0	0

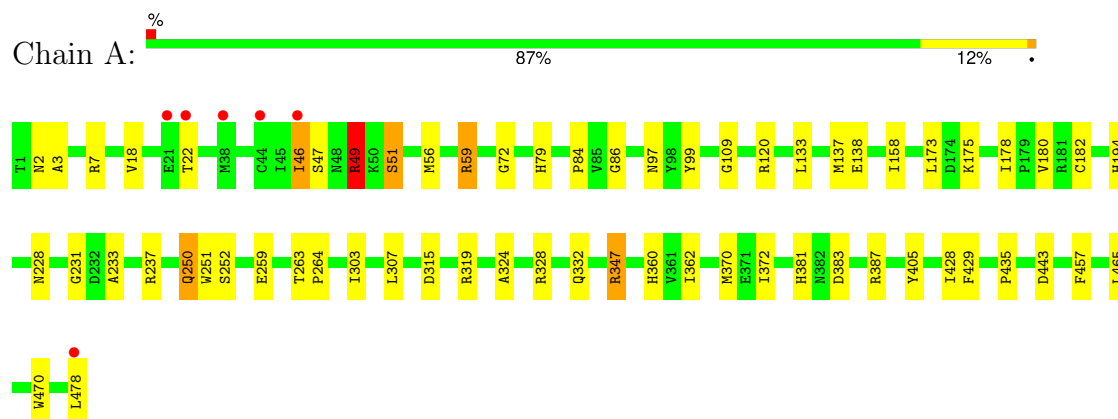
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	611	Total O 611 611	0	0
9	B	810	Total O 810 810	0	0
9	C	595	Total O 595 595	0	0
9	D	824	Total O 824 824	0	0

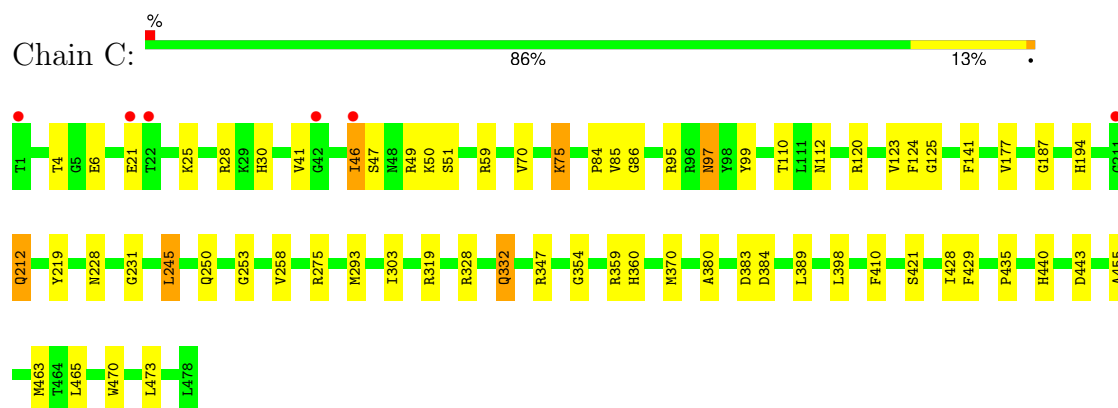
3 Residue-property plots

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.

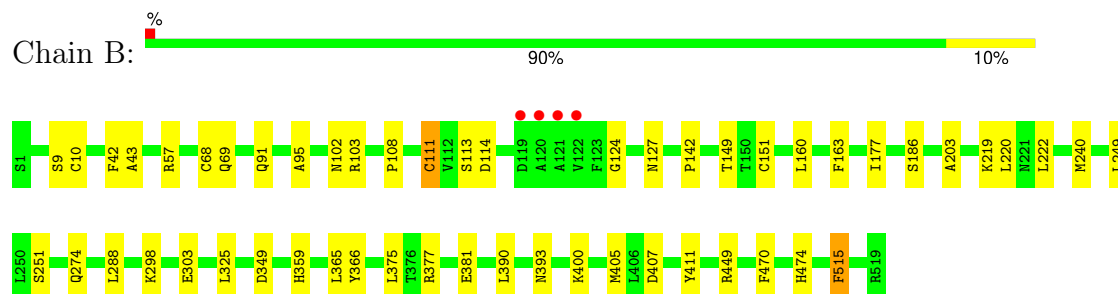
• Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



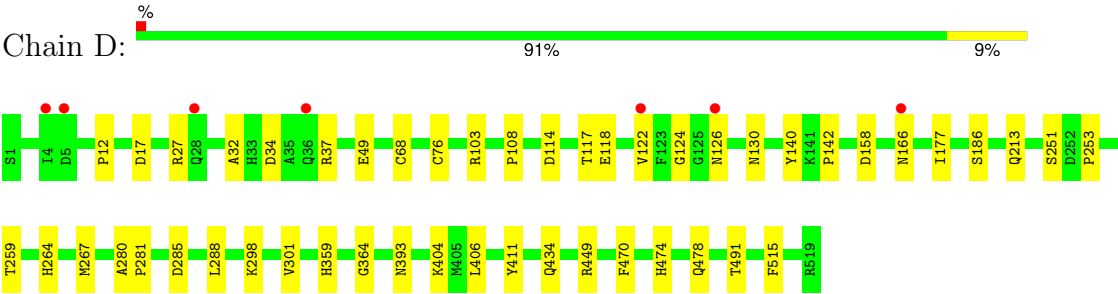
• Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



• Molecule 2: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



● Molecule 2: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.03Å 74.90Å 162.12Å 90.00° 122.80° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 50.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-1.60) 98.3 (50.00-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.155 , 0.197 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18565	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 3.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFM, CLF, HCA, CL, EDO, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.87	0/3815	1.58	36/5165 (0.7%)
1	C	0.86	0/3811	1.60	43/5158 (0.8%)
2	B	0.86	0/4192	1.54	28/5686 (0.5%)
2	D	0.86	0/4186	1.52	32/5679 (0.6%)
All	All	0.86	0/16004	1.56	139/21688 (0.6%)

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
1	A	0	3
1	C	0	4
2	B	0	1
All	All	0	8

There are no bond length outliers.

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	449	ARG	CD-NE-CZ	16.01	146.82	124.40
1	C	383	ASP	CA-CB-CG	9.50	122.10	112.60
1	A	347	ARG	CD-NE-CZ	8.74	136.63	124.40
1	C	332	GLN	OE1-CD-NE2	-8.68	113.92	122.60
1	A	178	ILE	N-CA-C	8.14	116.31	107.60
1	C	303	ILE	O-C-N	8.08	129.70	121.87
2	D	213	GLN	O-C-N	7.99	126.06	121.27
1	A	120	ARG	CA-CB-CG	7.91	129.91	114.10
2	D	449	ARG	CD-NE-CZ	7.73	135.23	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	27	ARG	CD-NE-CZ	7.68	135.15	124.40
1	C	46	ILE	O-C-N	7.66	131.20	123.00
1	A	328	ARG	CD-NE-CZ	7.55	134.97	124.40
2	D	124	GLY	N-CA-C	-7.25	103.54	112.68
1	A	2	ASN	OD1-CG-ND2	7.19	129.79	122.60
1	C	28	ARG	CD-NE-CZ	7.09	134.32	124.40
1	C	30	HIS	O-C-N	-6.99	113.75	122.35
1	C	25	LYS	CA-C-O	-6.98	113.15	120.55
1	A	137	MET	CA-C-O	6.97	128.13	120.82
1	C	410	PHE	CA-CB-CG	6.86	120.66	113.80
1	A	383	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	175	LYS	CA-C-O	-6.83	114.22	120.50
1	C	50	LYS	CA-C-N	-6.82	107.00	121.32
1	C	50	LYS	C-N-CA	-6.82	107.00	121.32
2	D	76	CYS	O-C-N	6.81	129.34	122.12
2	D	478	GLN	CG-CD-NE2	-6.77	106.24	116.40
2	D	470	PHE	CA-CB-CG	6.75	120.55	113.80
2	B	113	SER	CA-C-N	-6.75	112.08	122.60
2	B	113	SER	C-N-CA	-6.75	112.08	122.60
1	A	49	ARG	CD-NE-CZ	6.75	133.84	124.40
2	D	103	ARG	NE-CZ-NH2	-6.73	113.14	119.20
2	B	102	ASN	CA-CB-CG	6.70	119.30	112.60
1	C	429	PHE	CA-CB-CG	-6.68	107.11	113.80
2	B	407	ASP	CB-CG-OD2	6.66	133.72	118.40
2	D	434	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	A	332	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	C	410	PHE	CA-C-O	6.55	127.70	120.82
1	A	51[A]	SER	CA-C-O	-6.55	114.42	121.56
1	A	51[B]	SER	CA-C-O	-6.55	114.42	121.56
2	B	124	GLY	N-CA-C	-6.36	105.16	112.29
1	C	46	ILE	CA-C-O	-6.32	113.95	121.28
1	A	429	PHE	CA-CB-CG	-6.31	107.49	113.80
1	A	478	LEU	CA-C-O	-6.30	110.09	120.80
2	D	114	ASP	CA-CB-CG	6.24	118.84	112.60
2	D	126	ASN	OD1-CG-ND2	-6.23	116.37	122.60
2	B	114	ASP	CA-CB-CG	6.16	118.76	112.60
2	B	515	PHE	CA-CB-CG	6.11	119.91	113.80
2	D	130	ASN	O-C-N	-6.09	115.80	122.07
2	D	434	GLN	CA-CB-CG	-6.07	101.96	114.10
1	A	86	GLY	O-C-N	-5.98	114.92	122.70
1	C	328	ARG	CD-NE-CZ	5.97	132.75	124.40
1	C	21	GLU	N-CA-C	5.96	118.26	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	HIS	CA-CB-CG	-5.91	107.89	113.80
2	B	95	ALA	O-C-N	5.91	128.38	122.12
1	C	194	HIS	O-C-N	5.91	128.15	122.07
2	B	393	ASN	CA-CB-CG	5.88	118.48	112.60
2	B	163	PHE	CA-CB-CG	5.88	119.68	113.80
1	C	51	SER	N-CA-C	5.85	118.45	110.55
1	C	97	ASN	CA-CB-CG	5.85	118.45	112.60
1	C	319	ARG	O-C-N	-5.85	116.05	122.07
1	C	4	THR	CA-C-N	5.84	126.57	120.03
1	C	4	THR	C-N-CA	5.84	126.57	120.03
1	C	440	HIS	CA-CB-CG	5.82	119.62	113.80
2	D	478	GLN	CG-CD-OE1	5.82	132.44	120.80
1	C	258	VAL	O-C-N	-5.80	116.23	121.91
1	A	324	ALA	O-C-N	5.79	128.26	122.12
1	C	25	LYS	O-C-N	5.78	128.25	122.12
1	C	250	GLN	CG-CD-NE2	5.78	125.07	116.40
2	B	69	GLN	OE1-CD-NE2	5.74	128.34	122.60
1	C	51	SER	N-CA-CB	-5.74	101.73	110.45
2	D	474	HIS	CA-CB-CG	-5.71	108.09	113.80
1	A	307	LEU	O-C-N	5.70	128.16	122.12
1	A	137	MET	O-C-N	-5.69	116.21	122.07
1	C	187	GLY	CA-C-O	-5.63	114.90	122.33
2	D	285	ASP	O-C-N	5.61	128.90	123.29
1	A	319	ARG	CD-NE-CZ	5.60	132.24	124.40
1	A	180	VAL	CA-C-O	5.58	125.90	120.27
2	B	127	ASN	CA-CB-CG	-5.57	107.03	112.60
1	A	259	GLU	CB-CG-CD	-5.54	103.18	112.60
1	A	158	ILE	N-CA-C	-5.54	107.35	112.83
1	A	381	HIS	CA-CB-CG	5.52	119.32	113.80
1	C	421	SER	CA-C-O	-5.52	116.22	120.19
2	B	151	CYS	N-CA-CB	5.51	118.81	110.28
1	A	194	HIS	O-C-N	5.50	127.74	122.07
2	D	49	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	178	ILE	N-CA-CB	-5.50	104.08	111.40
1	C	59	ARG	CD-NE-CZ	-5.50	116.70	124.40
1	C	293	MET	O-C-N	5.48	129.52	123.33
2	B	349	ASP	CA-CB-CG	-5.47	107.13	112.60
1	A	387	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	C	86	GLY	O-C-N	-5.42	116.98	122.18
1	C	359	ARG	CD-NE-CZ	5.42	131.98	124.40
2	D	393	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	A	47	SER	O-C-N	-5.41	117.58	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	515	PHE	CA-CB-CG	5.41	119.21	113.80
2	B	103	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	250	GLN	CB-CA-C	-5.34	101.60	110.14
1	A	303	ILE	O-C-N	5.33	127.13	121.91
1	C	410	PHE	O-C-N	-5.33	116.58	122.07
2	D	406	LEU	CA-C-O	-5.32	114.79	120.42
1	C	141	PHE	CA-CB-CG	-5.31	108.49	113.80
1	C	75	LYS	N-CA-C	5.30	117.97	111.82
2	B	42	PHE	CA-CB-CG	-5.28	108.52	113.80
1	C	125	GLY	O-C-N	5.28	127.38	122.47
2	D	264	HIS	CA-CB-CG	-5.27	108.53	113.80
1	C	389	LEU	CA-C-O	5.27	123.18	118.33
1	A	457	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	175	LYS	O-C-N	5.26	125.07	121.71
1	C	398	LEU	O-C-N	-5.25	117.18	123.27
2	D	158	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	47	SER	O-C-N	-5.23	116.80	122.92
2	D	130	ASN	CA-C-O	5.21	126.30	120.82
2	D	103	ARG	NE-CZ-NH1	5.21	126.71	121.50
2	D	17	ASP	O-C-N	5.21	127.64	122.12
2	B	405	MET	O-C-N	-5.20	116.61	122.12
1	A	315	ASP	CA-C-O	5.17	126.84	121.36
2	D	118	GLU	CA-C-O	-5.17	115.05	120.63
2	B	449	ARG	O-C-N	5.16	127.39	122.07
2	B	470	PHE	CA-CB-CG	5.16	118.96	113.80
2	B	111	CYS	CA-C-N	-5.15	115.61	122.77
2	B	111	CYS	C-N-CA	-5.15	115.61	122.77
2	B	240	MET	CA-C-O	-5.15	114.28	120.10
2	B	274	GLN	CA-C-O	-5.14	115.10	120.55
1	A	72	GLY	O-C-N	-5.13	116.64	121.77
2	B	220	LEU	CA-C-O	-5.11	115.19	120.70
1	C	6	GLU	CA-CB-CG	-5.10	103.90	114.10
2	D	17	ASP	CA-C-O	-5.10	115.12	120.63
1	C	41	VAL	CA-C-O	-5.10	114.75	120.25
2	D	364	GLY	N-CA-C	-5.10	101.75	112.04
2	D	37	ARG	O-C-N	5.07	127.93	122.15
2	B	203	ALA	O-C-N	5.06	127.92	122.15
2	D	259	THR	CA-C-N	5.06	124.96	119.85
2	D	259	THR	C-N-CA	5.06	124.96	119.85
2	B	325	LEU	O-C-N	5.05	128.49	122.27
1	C	70	VAL	N-CA-C	5.04	115.71	110.82
2	D	301	VAL	O-C-N	5.04	126.76	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	ALA	O-C-N	-5.03	116.79	122.12
1	A	46	ILE	CA-C-O	-5.02	116.40	121.67
1	A	59	ARG	CD-NE-CZ	-5.01	117.39	124.40
1	C	85	VAL	N-CA-C	5.01	119.05	112.04

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	GLY	Mainchain
1	A	182	CYS	Mainchain
1	A	231	GLY	Mainchain
2	B	303	GLU	Mainchain
1	C	177	VAL	Mainchain
1	C	231	GLY	Mainchain
1	C	354	GLY	Mainchain
1	C	95	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	3709	0	3567	22	0
1	C	3716	0	3593	25	0
2	B	4067	0	3926	21	0
2	D	4060	0	3918	16	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	14	0	6	1	0
4	C	14	0	6	1	0
5	A	17	0	0	0	0
5	C	17	0	0	0	0
6	A	17	0	0	0	0
6	C	17	0	0	0	0
7	A	20	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	24	0	36	6	0
7	C	4	0	6	0	0
7	D	20	0	30	2	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	611	0	0	4	0
9	B	810	0	0	5	0
9	C	595	0	0	8	0
9	D	824	0	0	3	0
All	All	18565	0	15118	84	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 3.

All (84) 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)
2:B:222:LEU:HB2	2:B:249:LEU:HD23	1.62	0.81
2:D:32:ALA:HB3	7:D:2919:EDO:H12	1.65	0.79
1:A:99:TYR:HE2	9:A:3451:HOH:O	1.70	0.73
7:B:2904:EDO:H12	9:B:3702:HOH:O	1.90	0.69
1:A:347:ARG:HG3	1:A:465:LEU:HD21	1.75	0.69
1:A:347:ARG:HH11	1:A:465:LEU:HD21	1.56	0.68
1:A:428:ILE:HG13	2:B:108:PRO:HB3	1.77	0.67
1:C:46:ILE:HD12	1:C:49:ARG:HD2	1.80	0.64
1:C:99:TYR:HE1	9:C:1881:HOH:O	1.81	0.62
2:B:400:LYS:HE2	9:B:3411:HOH:O	1.99	0.62
2:B:68:CYS:HB2	2:B:186:SER:HB2	1.82	0.61
1:C:120:ARG:HA	1:C:123:VAL:HG22	1.82	0.61
2:D:166:ASN:HB3	9:D:3664:HOH:O	2.00	0.60
1:C:347:ARG:HG3	1:C:465:LEU:HD21	1.85	0.59
7:B:2907:EDO:H21	2:D:491:THR:OG1	2.02	0.58
1:C:123:VAL:HG23	1:C:124:PHE:CD2	2.38	0.58
1:A:49:ARG:HD3	9:A:3332:HOH:O	2.03	0.58
7:A:2910:EDO:H12	9:A:3449:HOH:O	2.04	0.57
1:A:347:ARG:HB2	1:A:370:MET:HE3	1.87	0.56
2:B:149:THR:HG23	2:B:160:LEU:HD11	1.88	0.56
2:D:68:CYS:HB2	2:D:186:SER:HB2	1.86	0.56
1:A:347:ARG:HH11	1:A:465:LEU:CD2	2.18	0.56
7:A:2910:EDO:H12	9:A:3451:HOH:O	2.05	0.56
4:A:501:HCA:O2	4:A:501:HCA:O7	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365[A]:LEU:HD13	2:B:375:LEU:HD23	1.89	0.54
1:C:455:ALA:HB2	9:C:1875:HOH:O	2.07	0.54
1:C:46:ILE:HD12	1:C:49:ARG:CD	2.37	0.54
1:A:46:ILE:HD12	1:A:49:ARG:HD2	1.90	0.53
2:B:57:ARG:O	7:B:2906:EDO:H12	2.08	0.53
1:C:435:PRO:HA	1:C:470:TRP:CZ2	2.44	0.53
4:C:501:HCA:O2	4:C:501:HCA:O7	2.26	0.53
2:D:32:ALA:CB	7:D:2919:EDO:H12	2.39	0.52
1:A:362:ILE:HG12	1:A:372:ILE:HG13	1.91	0.51
1:C:347:ARG:HB2	1:C:370:MET:HE3	1.93	0.51
1:C:428:ILE:HG13	2:D:108:PRO:HB3	1.93	0.50
2:D:288:LEU:HD11	2:D:298:LYS:HA	1.93	0.50
1:C:219:TYR:HB3	1:C:245:LEU:HD12	1.93	0.50
2:B:219:LYS:HE3	9:B:3595:HOH:O	2.12	0.49
2:B:288:LEU:HD11	2:B:298:LYS:HA	1.94	0.49
1:A:3:ALA:O	1:A:7:ARG:HG3	2.12	0.49
1:A:138:GLU:HG2	1:A:173:LEU:HD22	1.95	0.48
1:A:435:PRO:HA	1:A:470:TRP:CZ2	2.48	0.48
1:A:133:LEU:HD23	1:A:133:LEU:C	2.37	0.48
1:A:51[A]:SER:OG	1:A:59:ARG:HD2	2.12	0.48
1:A:18:VAL:HG11	1:A:405:TYR:CE2	2.49	0.48
2:D:68:CYS:HB2	2:D:186:SER:CB	2.44	0.47
7:B:2907:EDO:H11	2:D:491:THR:HG21	1.95	0.47
1:A:51[B]:SER:OG	2:B:91:GLN:NE2	2.42	0.47
2:D:140:TYR:CD1	2:D:267:MET:HE1	2.50	0.46
1:A:228:ASN:HA	1:A:233:ALA:H	1.81	0.46
1:C:110:THR:HG23	9:C:1881:HOH:O	2.16	0.46
2:D:142:PRO:O	2:D:177[A]:ILE:HD12	2.16	0.46
1:A:237:ARG:HD2	1:A:250:GLN:OE1	2.16	0.45
1:C:99:TYR:HE2	9:C:1818:HOH:O	2.00	0.45
1:C:332:GLN:NE2	9:C:1875:HOH:O	2.49	0.45
2:B:365[A]:LEU:CD1	2:B:375:LEU:HD23	2.47	0.44
2:D:359:HIS:HE1	2:D:411:TYR:OH	1.99	0.44
2:B:474:HIS:O	7:B:2907:EDO:H12	2.17	0.44
7:B:2907:EDO:C2	2:D:491:THR:OG1	2.66	0.43
2:D:267:MET:HE2	9:D:3457:HOH:O	2.17	0.43
2:D:280:ALA:N	2:D:281:PRO:CD	2.81	0.43
2:B:359:HIS:HE1	2:B:411:TYR:OH	2.01	0.42
2:D:117:THR:HG22	9:D:3616:HOH:O	2.18	0.42
1:A:251:TRP:HA	1:A:252:SER:HA	1.76	0.42
2:B:381:GLU:HG3	9:B:3486:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLN:HB3	9:C:1910:HOH:O	2.19	0.42
1:A:263:THR:N	1:A:264:PRO:CD	2.82	0.42
2:B:377:ARG:HG2	2:B:381:GLU:OE2	2.19	0.42
1:C:347:ARG:NH2	9:C:1784:HOH:O	2.52	0.42
1:C:380:ALA:HB1	1:C:384:ASP:HB2	2.01	0.42
1:C:428:ILE:CD1	9:C:1665:HOH:O	2.68	0.41
2:B:142:PRO:O	2:B:177[A]:ILE:HD12	2.20	0.41
2:B:515:PHE:HB3	9:B:3701:HOH:O	2.20	0.41
2:B:9:SER:O	2:B:10:CYS:C	2.64	0.41
1:C:112:ASN:C	1:C:112:ASN:ND2	2.79	0.41
1:C:275:ARG:HD2	1:C:384:ASP:OD2	2.21	0.41
2:B:359:HIS:CG	1:C:463:MET:HG3	2.55	0.41
2:B:366:TYR:HA	2:B:390:LEU:O	2.21	0.40
1:C:228:ASN:HB2	1:C:253:GLY:HA3	2.03	0.40
1:A:56:MET:HG3	2:B:111:CYS:O	2.22	0.40
1:C:112:ASN:C	1:C:112:ASN:HD22	2.30	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	480/478 (100%)	464 (97%)	16 (3%)	0	100	100
1	C	478/478 (100%)	461 (96%)	17 (4%)	0	100	100
2	B	523/519 (101%)	512 (98%)	10 (2%)	1 (0%)	43	24
2	D	523/519 (101%)	513 (98%)	9 (2%)	1 (0%)	43	24
All	All	2004/1994 (100%)	1950 (97%)	52 (3%)	2 (0%)	48	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER
2	D	251	SER

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	380/397 (96%)	375 (99%)	5 (1%)	61	40
1	C	379/397 (96%)	373 (98%)	6 (2%)	55	33
2	B	429/442 (97%)	429 (100%)	0	100	100
2	D	434/442 (98%)	429 (99%)	5 (1%)	63	43
All	All	1622/1678 (97%)	1606 (99%)	16 (1%)	68	50

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	49	ARG
1	A	97	ASN
1	A	360	HIS
1	A	443	ASP
1	C	97	ASN
1	C	212	GLN
1	C	245	LEU
1	C	360	HIS
1	C	443	ASP
1	C	473	LEU
2	D	12	PRO
2	D	34	ASP
2	D	122	VAL
2	D	253	PRO
2	D	404	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	ASN
2	B	82	ASN
2	B	91	GLN
2	B	126	ASN
2	B	290	GLN
2	B	359	HIS
2	B	399	GLN
1	C	112	ASN
1	C	288	HIS
1	C	313	GLN
2	D	82	ASN
2	D	91	GLN
2	D	274	GLN
2	D	290	GLN
2	D	359	HIS
2	D	434	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 9 are monoatomic - leaving 25 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
7	EDO	B	2904	-	3,3,3	0.60	0	2,2,2	1.19	0
6	CLF	C	505[A]	1,2	0,24,24	-	-	-		
7	EDO	C	2914	-	3,3,3	0.30	0	2,2,2	0.44	0
7	EDO	D	2918	-	3,3,3	0.39	0	2,2,2	0.17	0
7	EDO	B	2903	-	3,3,3	0.41	0	2,2,2	0.66	0
4	HCA	A	501	5	13,13,13	3.00	7 (53%)	15,18,18	2.76	5 (33%)
7	EDO	B	2906	-	3,3,3	0.47	0	2,2,2	0.23	0
7	EDO	A	2911	-	3,3,3	0.38	0	2,2,2	0.11	0
7	EDO	B	2907	-	3,3,3	0.64	0	2,2,2	2.65	2 (100%)
7	EDO	A	2915	-	3,3,3	0.26	0	2,2,2	0.19	0
7	EDO	A	2912	-	3,3,3	0.34	0	2,2,2	0.42	0
6	CLF	A	505[B]	1,2	0,24,24	-	-	-		
5	CFM	A	503	4,1	0,24,24	-	-	-		
7	EDO	A	2910	-	3,3,3	0.51	0	2,2,2	0.82	0
7	EDO	B	2913	-	3,3,3	0.49	0	2,2,2	0.16	0
4	HCA	C	501	5	13,13,13	3.00	7 (53%)	15,18,18	3.28	8 (53%)
7	EDO	D	2917	-	3,3,3	0.67	0	2,2,2	0.07	0
7	EDO	D	2908	-	3,3,3	0.47	0	2,2,2	0.45	0
7	EDO	D	2916	-	3,3,3	0.60	0	2,2,2	0.05	0
6	CLF	C	505[B]	1,2	0,24,24	-	-	-		
6	CLF	A	505[A]	1,2	0,24,24	-	-	-		
7	EDO	A	2909	-	3,3,3	0.46	0	2,2,2	0.56	0
7	EDO	B	2905	-	3,3,3	0.11	0	2,2,2	0.41	0
7	EDO	D	2919	-	3,3,3	0.36	0	2,2,2	0.43	0
5	CFM	C	503	4,1	0,24,24	-	-	-		

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
7	EDO	B	2904	-	-	1/1/1/1	-
6	CLF	C	505[A]	1,2	-	-	0/12/10/10
7	EDO	C	2914	-	-	0/1/1/1	-
7	EDO	D	2918	-	-	0/1/1/1	-
7	EDO	B	2903	-	-	0/1/1/1	-
4	HCA	A	501	5	-	2/17/17/17	-
7	EDO	B	2906	-	-	1/1/1/1	-
7	EDO	A	2911	-	-	1/1/1/1	-
7	EDO	B	2907	-	-	1/1/1/1	-
7	EDO	A	2915	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	2912	-	-	0/1/1/1	-
6	CLF	A	505[B]	1,2	-	-	0/12/10/10
7	EDO	A	2910	-	-	0/1/1/1	-
7	EDO	B	2913	-	-	1/1/1/1	-
4	HCA	C	501	5	-	2/17/17/17	-
7	EDO	D	2917	-	-	0/1/1/1	-
7	EDO	D	2908	-	-	1/1/1/1	-
6	CLF	C	505[B]	1,2	-	-	0/12/10/10
6	CLF	A	505[A]	1,2	-	-	0/12/10/10
7	EDO	A	2909	-	-	0/1/1/1	-
7	EDO	B	2905	-	-	0/1/1/1	-
7	EDO	D	2919	-	-	1/1/1/1	-
7	EDO	D	2916	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	HCA	C2-C3	-5.63	1.47	1.54
4	C	501	HCA	C2-C1	5.19	1.66	1.50
4	C	501	HCA	O7-C3	5.05	1.52	1.43
4	C	501	HCA	C2-C3	-4.96	1.47	1.54
4	A	501	HCA	C2-C1	4.55	1.64	1.50
4	A	501	HCA	O7-C3	4.11	1.51	1.43
4	A	501	HCA	C3-C7	4.11	1.57	1.53
4	C	501	HCA	O6-C7	-3.41	1.18	1.30
4	A	501	HCA	O6-C7	-3.16	1.19	1.30
4	C	501	HCA	C3-C7	2.91	1.56	1.53
4	A	501	HCA	O3-C6	2.75	1.31	1.22
4	C	501	HCA	O5-C7	2.56	1.30	1.22
4	A	501	HCA	O5-C7	2.24	1.29	1.22
4	C	501	HCA	O3-C6	2.03	1.28	1.22

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	HCA	O2-C1-O1	7.05	141.45	123.33
4	C	501	HCA	O7-C3-C4	-6.65	98.25	108.88
4	A	501	HCA	O7-C3-C4	-5.65	99.85	108.88
4	A	501	HCA	O2-C1-O1	5.52	137.52	123.33
4	C	501	HCA	O1-C1-C2	-4.12	111.27	122.95
4	A	501	HCA	C4-C5-C6	3.99	122.01	112.77
4	A	501	HCA	O1-C1-C2	-3.54	112.93	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	HCA	C4-C5-C6	3.48	120.83	112.77
4	C	501	HCA	O6-C7-C3	3.16	119.20	113.14
7	B	2907	EDO	O1-C1-C2	3.02	135.40	112.39
4	C	501	HCA	O3-C6-C5	-2.83	114.12	123.09
4	A	501	HCA	O6-C7-C3	2.53	117.99	113.14
4	C	501	HCA	O7-C3-C7	-2.49	105.43	108.96
4	C	501	HCA	O2-C1-C2	-2.23	107.27	114.35
7	B	2907	EDO	O2-C2-C1	2.22	129.29	112.39

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	2919	EDO	O1-C1-C2-O2
7	B	2913	EDO	O1-C1-C2-O2
4	A	501	HCA	C7-C3-C4-C5
7	B	2904	EDO	O1-C1-C2-O2
7	B	2907	EDO	O1-C1-C2-O2
7	B	2906	EDO	O1-C1-C2-O2
7	D	2908	EDO	O1-C1-C2-O2
4	A	501	HCA	O1-C1-C2-C3
7	A	2911	EDO	O1-C1-C2-O2
4	C	501	HCA	O1-C1-C2-C3
4	C	501	HCA	O2-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2904	EDO	1	0
4	A	501	HCA	1	0
7	B	2906	EDO	1	0
7	B	2907	EDO	4	0
7	A	2910	EDO	2	0
4	C	501	HCA	1	0
7	D	2919	EDO	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	478/478 (100%)	0.03	6 (1%) 75 79	8, 15, 26, 36	4 (0%)
1	C	478/478 (100%)	0.58	6 (1%) 75 79	9, 17, 28, 38	2 (0%)
2	B	519/519 (100%)	-0.01	4 (0%) 82 86	7, 14, 25, 34	6 (1%)
2	D	519/519 (100%)	0.14	7 (1%) 75 79	7, 12, 23, 36	6 (1%)
All	All	1994/1994 (100%)	0.18	23 (1%) 76 80	7, 14, 26, 38	18 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	122	VAL	3.3
2	D	4	ILE	3.0
1	A	46	ILE	2.8
2	B	119	ASP	2.8
2	B	121	ALA	2.7
1	A	21	GLU	2.6
2	B	120	ALA	2.6
1	C	22	THR	2.6
2	D	28	GLN	2.6
2	D	5	ASP	2.4
2	D	36	GLN	2.3
1	A	38	MET	2.3
1	C	46	ILE	2.3
1	C	211	GLY	2.3
1	C	1	THR	2.2
1	C	42	GLY	2.2
1	C	21	GLU	2.2
2	D	166	ASN	2.1
1	A	478	LEU	2.1
1	A	22	THR	2.1
2	B	122	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	126	ASN	2.0
1	A	44	CYS	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	EDO	A	2910	4/4	0.77	0.23	29,30,32,33	0
7	EDO	B	2906	4/4	0.78	0.23	37,40,41,42	0
3	MG	B	3003	1/1	0.81	0.12	27,27,27,27	0
3	MG	D	3007	1/1	0.81	0.12	29,29,29,29	0
7	EDO	A	2915	4/4	0.83	0.18	25,31,31,31	0
7	EDO	D	2919	4/4	0.85	0.13	23,29,32,34	0
7	EDO	D	2918	4/4	0.86	0.14	16,25,27,28	0
7	EDO	B	2913	4/4	0.88	0.12	19,20,21,22	0
7	EDO	C	2914	4/4	0.88	0.11	23,23,23,24	0
7	EDO	B	2903	4/4	0.88	0.12	21,22,23,24	0
7	EDO	A	2912	4/4	0.88	0.12	28,29,30,35	0
7	EDO	B	2905	4/4	0.89	0.13	22,24,28,35	0
7	EDO	A	2911	4/4	0.90	0.10	28,28,32,32	0
7	EDO	D	2908	4/4	0.92	0.12	18,19,22,24	0
4	HCA	C	501	14/14	0.93	0.08	8,11,12,13	0
7	EDO	B	2904	4/4	0.93	0.11	17,18,22,22	0
7	EDO	A	2909	4/4	0.93	0.12	17,18,21,22	0
7	EDO	D	2917	4/4	0.93	0.10	14,17,18,20	0
3	MG	C	3005	1/1	0.93	0.06	16,16,16,16	0
7	EDO	B	2907	4/4	0.93	0.13	16,21,21,29	0
6	CLF	C	505[A]	15/15	0.94	0.08	8,10,11,13	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CLF	C	505[B]	15/15	0.94	0.08	8,10,11,11	2
3	MG	B	3004	1/1	0.94	0.07	24,24,24,24	0
3	MG	D	3006	1/1	0.95	0.06	9,9,9,9	0
5	CFM	C	503	17/17	0.95	0.07	9,11,12,13	0
8	CL	D	2901	1/1	0.95	0.06	14,14,14,14	0
3	MG	B	3002	1/1	0.96	0.05	9,9,9,9	0
7	EDO	D	2916	4/4	0.96	0.06	15,15,15,19	0
8	CL	B	2902	1/1	0.96	0.07	17,17,17,17	0
4	HCA	A	501	14/14	0.96	0.06	8,11,13,13	0
3	MG	A	3001	1/1	0.97	0.09	16,16,16,16	0
5	CFM	A	503	17/17	0.98	0.05	9,10,11,12	0
6	CLF	A	505[A]	15/15	0.98	0.05	9,12,13,14	2
6	CLF	A	505[B]	15/15	0.98	0.05	9,12,13,15	2

6.5 Other polymers [i](#)

There are no such residues in this entry.