



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:45 PM UTC

PDB ID : 1QGU / pdb_00001qgu
Title : NITROGENASE MO-FE PROTEIN FROM KLEBSIELLA PNEUMONIAE,
DITHIONITE-REDUCED STATE
Authors : Mayer, S.M.; Lawson, D.M.; Gormal, C.A.; Roe, S.M.; Smith, B.E.
Deposited on : 1999-05-06
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

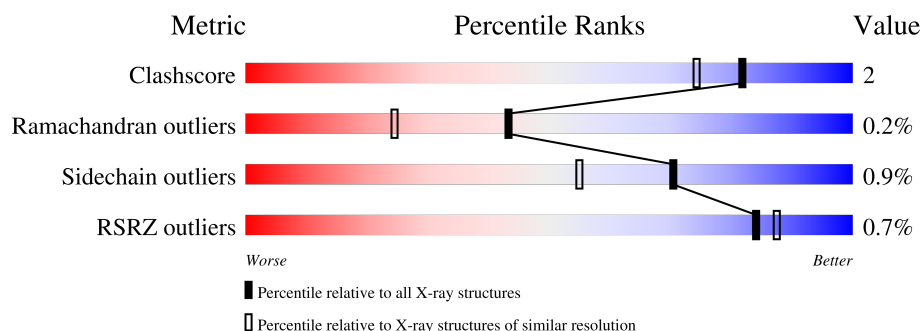
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	89% 10% .
2	B	519	90% 9% .
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	D	2784	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18462 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
			3700	2357	631	688	24			
1	C	478	Total	C	N	O	S	0	4	0
			3712	2365	631	692	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	10	0
			4069	2598	680	760	31			
2	D	519	Total	C	N	O	S	0	3	0
			4047	2582	679	756	30			

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

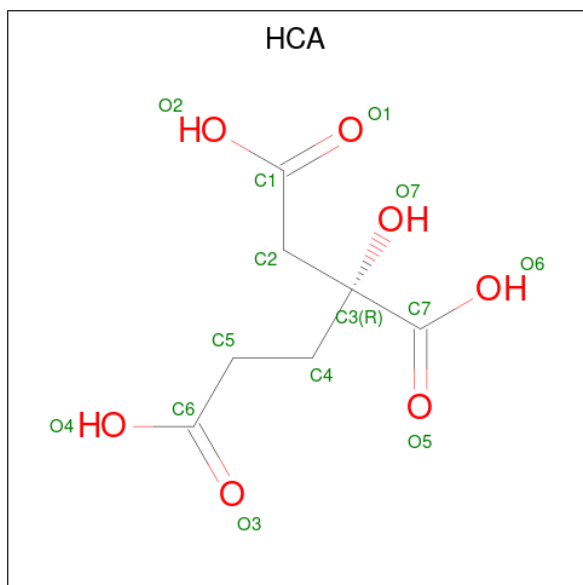
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	3	Total	Mg	0	0
			3	3		
3	C	1	Total	Mg	0	0
			1	1		

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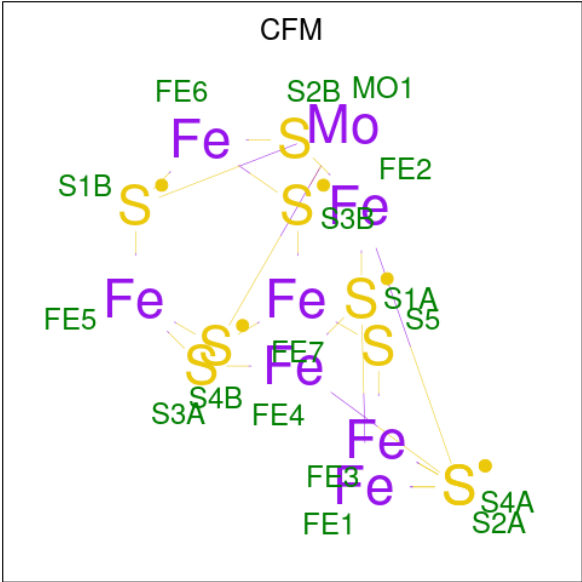
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		

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



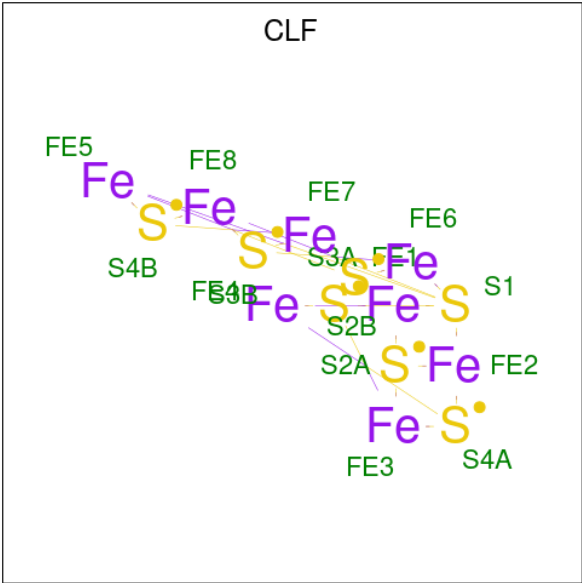
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		

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



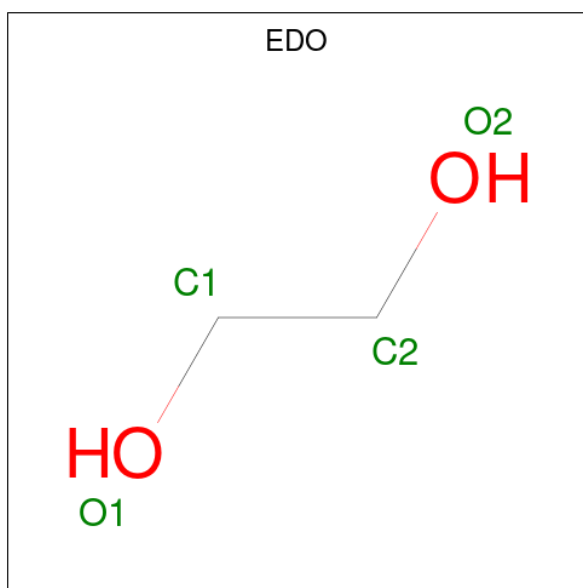
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- 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	0
			15	8	7		
6	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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	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		
7	D	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	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

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

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

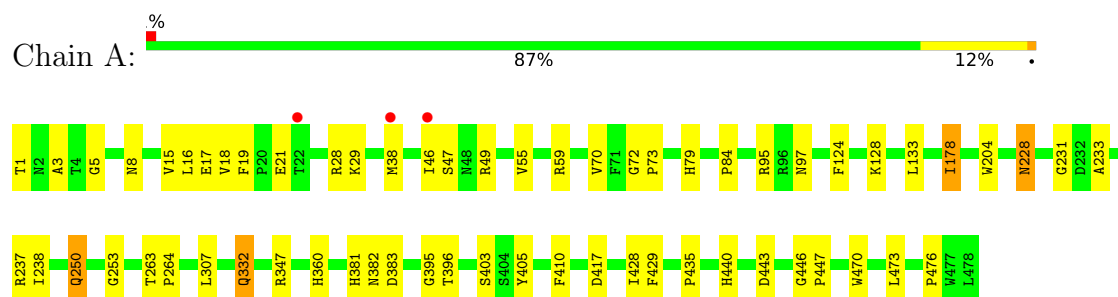
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	606	Total	O	0	0
			606	606		
9	B	794	Total	O	0	0
			794	794		
9	C	571	Total	O	0	0
			571	571		
9	D	798	Total	O	0	0
			798	798		

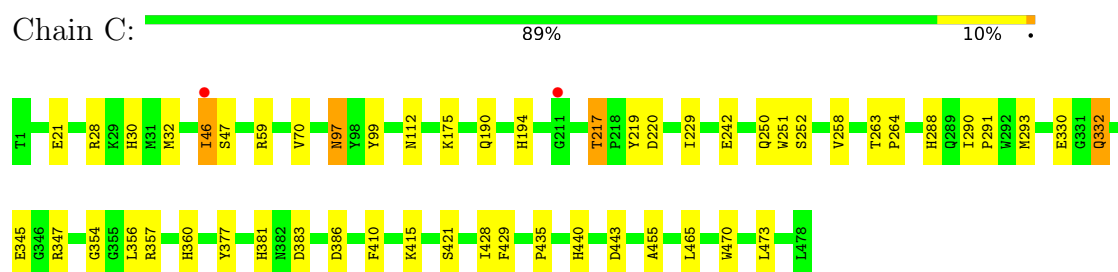
3 Residue-property plots

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.

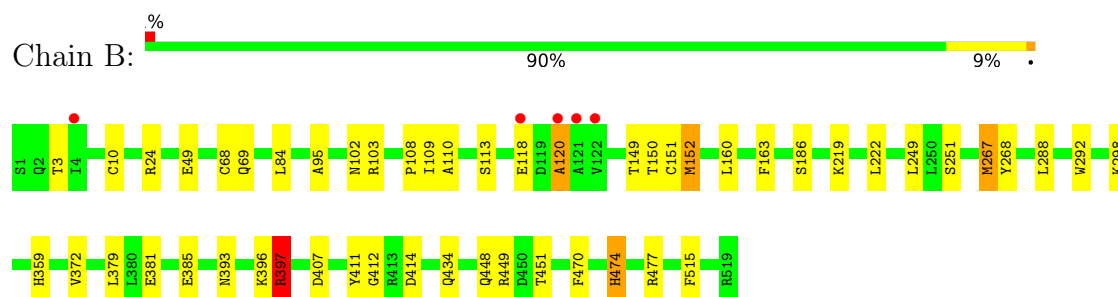
• Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



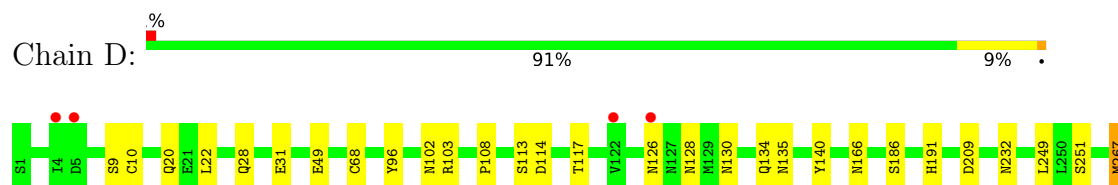
• Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



• 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	204.03Å 75.30Å 163.01Å 90.00° 122.61° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 50.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-1.60) 95.4 (50.00-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.156 , 0.199 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.5	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	0.97	EDS
Total number of atoms	18462	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 3.33% 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: CLF, CFM, MG, CL, HCA, EDO

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	0.89	0/3803	1.55	27/5153 (0.5%)
1	C	0.89	0/3813	1.61	38/5165 (0.7%)
2	B	0.91	0/4215	1.58	35/5717 (0.6%)
2	D	0.89	0/4159	1.50	32/5643 (0.6%)
All	All	0.89	0/15990	1.56	132/21678 (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	5
1	C	0	2
2	B	0	2
2	D	0	1
All	All	0	10

There are no bond length outliers.

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	ARG	NE-CZ-NH2	18.62	135.96	119.20
2	B	449	ARG	CD-NE-CZ	18.55	150.37	124.40
2	D	434	GLN	O-C-N	-12.38	115.83	121.53
1	C	332	GLN	OE1-CD-NE2	-10.41	112.19	122.60
2	B	397	ARG	NE-CZ-NH1	-9.27	112.23	121.50
1	A	47	SER	O-C-N	-8.76	114.07	123.26
1	A	332	GLN	OE1-CD-NE2	-8.68	113.92	122.60
1	C	28	ARG	CD-NE-CZ	8.27	135.98	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ASP	CA-CB-CG	8.05	120.65	112.60
2	B	24	ARG	CD-NE-CZ	8.00	135.60	124.40
2	B	102	ASN	CA-CB-CG	7.93	120.53	112.60
2	D	515	PHE	CA-CB-CG	7.54	121.34	113.80
2	D	102	ASN	CA-CB-CG	7.37	119.97	112.60
2	B	24	ARG	NE-CZ-NH2	-7.36	112.57	119.20
1	A	410	PHE	CA-CB-CG	7.35	121.15	113.80
2	D	232	ASN	OD1-CG-ND2	7.34	129.94	122.60
1	A	178[A]	ILE	N-CA-C	7.31	115.42	107.60
1	A	178[B]	ILE	N-CA-C	7.31	115.42	107.60
2	D	434	GLN	CB-CA-C	-7.29	106.03	111.20
1	A	124	PHE	CA-CB-CG	-7.06	106.74	113.80
2	B	407	ASP	CB-CG-OD2	7.03	134.57	118.40
2	B	103	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	C	383	ASP	CA-CB-CG	6.94	119.54	112.60
2	D	470	PHE	CA-CB-CG	6.76	120.56	113.80
2	D	249	LEU	CA-C-O	-6.66	113.46	121.05
2	D	114	ASP	CA-CB-CG	6.61	119.20	112.60
1	C	290	ILE	CA-C-O	-6.53	114.44	119.20
1	C	194	HIS	O-C-N	6.44	128.71	122.07
1	C	386	ASP	CA-CB-CG	6.42	119.03	112.60
1	A	440	HIS	CA-CB-CG	6.42	120.22	113.80
2	B	113	SER	CA-C-N	-6.36	112.68	122.60
2	B	113	SER	C-N-CA	-6.36	112.68	122.60
1	C	440	HIS	CA-CB-CG	6.34	120.14	113.80
1	C	97	ASN	CA-CB-CG	6.34	118.94	112.60
1	C	112	ASN	OD1-CG-ND2	-6.34	116.26	122.60
2	D	130	ASN	O-C-N	-6.32	115.56	122.07
1	C	410	PHE	CA-CB-CG	6.25	120.05	113.80
2	D	31	GLU	CA-C-O	6.24	129.08	121.84
2	B	69	GLN	OE1-CD-NE2	6.23	128.83	122.60
2	B	379	LEU	CA-C-O	-6.13	114.05	120.55
1	A	396	THR	CA-C-O	6.08	127.97	121.16
1	A	79	HIS	CA-CB-CG	-6.04	107.75	113.80
2	D	474	HIS	CA-CB-CG	-5.99	107.81	113.80
1	C	258	VAL	O-C-N	-5.96	116.06	121.91
2	B	434	GLN	OE1-CD-NE2	5.95	128.55	122.60
1	C	30	HIS	O-C-N	-5.94	115.21	122.34
1	A	21	GLU	N-CA-C	5.88	117.69	111.28
1	C	190	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	A	59	ARG	CD-NE-CZ	-5.86	116.19	124.40
1	C	46	ILE	CA-C-O	-5.84	114.50	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	GLU	CB-CG-CD	5.83	122.50	112.60
2	D	103	ARG	NE-CZ-NH2	-5.83	113.96	119.20
2	B	515	PHE	CA-CB-CG	5.81	119.61	113.80
1	C	429	PHE	CA-CB-CG	-5.78	108.02	113.80
1	C	229	ILE	O-C-N	-5.76	116.03	122.66
1	A	95	ARG	CG-CD-NE	5.76	124.67	112.00
2	B	397	ARG	NH1-CZ-NH2	-5.75	111.82	119.30
2	B	109	ILE	O-C-N	5.75	128.15	122.97
2	B	396	LYS	CA-C-O	-5.72	113.39	119.97
2	D	434	GLN	CB-CG-CD	-5.72	102.88	112.60
2	D	406	LEU	O-C-N	5.71	128.18	122.12
1	C	410	PHE	CA-C-O	5.71	126.82	120.82
1	C	250	GLN	CG-CD-NE2	5.71	124.96	116.40
1	A	382	ASN	CA-C-O	-5.69	113.67	120.10
1	A	381	HIS	CA-CB-CG	5.68	119.48	113.80
2	B	118	GLU	N-CA-C	5.66	120.70	111.37
2	D	381	GLU	CB-CG-CD	5.65	122.21	112.60
1	C	175	LYS	O-C-N	5.64	125.80	121.85
1	C	332	GLN	CA-CB-CG	5.64	125.38	114.10
1	C	421	SER	CA-C-O	-5.64	116.13	120.19
2	D	126	ASN	O-C-N	-5.63	115.73	122.15
1	C	356	LEU	CA-C-O	5.62	128.55	120.51
1	C	21	GLU	N-CA-C	5.61	118.12	111.33
2	B	163	PHE	CA-C-O	5.59	126.35	120.42
1	A	429	PHE	CA-CB-CG	-5.56	108.24	113.80
2	D	113	SER	CA-C-N	-5.56	113.93	122.60
2	D	113	SER	C-N-CA	-5.56	113.93	122.60
2	B	393	ASN	CA-CB-CG	5.56	118.16	112.60
1	C	288	HIS	CA-C-N	5.56	130.02	122.07
1	C	288	HIS	C-N-CA	5.56	130.02	122.07
2	B	151	CYS	O-C-N	5.54	128.70	122.22
2	D	135	ASN	O-C-N	5.54	128.47	122.15
1	C	415	LYS	CA-C-O	5.50	124.71	120.48
2	B	49	GLU	CB-CG-CD	5.49	121.92	112.60
2	D	49	GLU	CB-CG-CD	5.48	121.91	112.60
2	D	130	ASN	CA-C-O	5.47	126.56	120.82
1	A	59	ARG	N-CA-C	5.45	117.77	110.35
2	D	128	ASN	CA-C-O	-5.44	114.79	120.55
2	D	96	TYR	CA-C-O	-5.42	114.68	120.42
1	C	70	VAL	N-CA-C	5.39	116.05	110.82
1	A	70	VAL	N-CA-C	5.38	116.04	110.82
1	C	330	GLU	CB-CG-CD	5.38	121.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	166	ASN	OD1-CG-ND2	-5.38	117.22	122.60
2	B	95	ALA	O-C-N	5.37	127.81	122.12
1	A	228	ASN	OD1-CG-ND2	-5.36	117.24	122.60
2	D	20	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	C	455	ALA	O-C-N	5.35	127.80	122.12
1	C	293	MET	CA-C-O	-5.34	115.01	120.99
1	A	28	ARG	CD-NE-CZ	5.34	131.87	124.40
1	A	38	MET	N-CA-C	5.33	118.17	110.28
2	B	474	HIS	CA-CB-CG	-5.33	108.47	113.80
2	B	385	GLU	CB-CG-CD	-5.32	103.56	112.60
2	B	163	PHE	CA-CB-CG	5.32	119.12	113.80
1	A	238	ILE	CA-C-O	-5.30	115.44	120.95
1	C	381	HIS	CA-CB-CG	5.30	119.10	113.80
1	C	377	TYR	CA-CB-CG	5.29	123.42	113.90
2	D	134	GLN	O-C-N	-5.27	116.64	122.07
1	C	47	SER	O-C-N	-5.25	116.78	122.92
2	B	451	THR	O-C-N	-5.22	116.20	122.15
2	D	126	ASN	OD1-CG-ND2	-5.21	117.39	122.60
2	D	191	HIS	CA-CB-CG	-5.21	108.59	113.80
2	B	407	ASP	OD1-CG-OD2	-5.18	110.46	122.90
1	C	357	ARG	N-CA-C	5.18	120.72	113.57
2	B	219	LYS	CA-C-O	5.14	127.46	121.44
2	B	470	PHE	CA-CB-CG	5.14	118.94	113.80
2	B	292	TRP	CA-C-O	-5.14	114.29	120.10
2	D	406	LEU	CA-C-O	-5.14	115.10	120.55
1	C	291	PRO	CA-C-O	-5.13	115.54	121.95
2	B	151	CYS	CA-C-O	-5.12	114.31	120.10
2	B	412	GLY	CA-C-O	-5.12	114.39	119.04
2	D	478	GLN	CG-CD-OE1	5.10	131.00	120.80
1	A	8	ASN	CA-C-O	5.10	125.82	120.42
1	C	59	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	A	307	LEU	O-C-N	5.09	127.52	122.12
2	B	412	GLY	O-C-N	5.08	126.80	121.97
1	A	128	LYS	O-C-N	5.06	127.92	122.15
1	C	32	MET	O-C-N	-5.05	117.59	122.99
1	A	250	GLN	CB-CG-CD	5.04	121.17	112.60
1	A	473	LEU	CA-C-O	-5.04	115.08	120.42
2	B	372	VAL	CA-C-O	-5.04	115.71	120.95
2	D	301	VAL	O-C-N	5.03	126.75	121.87
2	D	209	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	GLU	Mainchain
1	A	231	GLY	Mainchain
1	A	3	ALA	Mainchain
1	A	395	GLY	Mainchain
1	A	476	PRO	Mainchain
2	B	120	ALA	Mainchain
2	B	3	THR	Mainchain
1	C	354	GLY	Mainchain
1	C	46	ILE	Mainchain
2	D	279	GLU	Mainchain

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	3700	0	3564	21	0
1	C	3712	0	3576	11	0
2	B	4069	0	3924	20	0
2	D	4047	0	3910	23	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	0	0
5	A	17	0	0	0	0
5	C	17	0	0	0	0
6	A	15	0	0	1	0
6	C	15	0	0	0	0
7	A	20	0	30	0	0
7	B	16	0	23	1	0
7	C	4	0	6	0	0
7	D	24	0	36	10	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	606	0	0	2	0
9	B	794	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	571	0	0	4	0
9	D	798	0	0	5	0
All	All	18462	0	15081	77	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 2.

All (77) 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:D:28:GLN:HA	7:D:2788:EDO:C1	2.02	0.90
2:D:491:THR:OG1	7:D:2784:EDO:H21	1.75	0.87
2:B:84:LEU:HD13	2:B:267[B]:MET:HE1	1.60	0.81
2:D:28:GLN:HA	7:D:2788:EDO:H12	1.64	0.80
1:A:178[A]:ILE:HD12	1:A:204:TRP:HB3	1.70	0.72
2:B:222:LEU:HB2	2:B:249:LEU:HD23	1.69	0.72
2:B:414:ASP:HB2	9:B:3639:HOH:O	1.92	0.69
2:D:28:GLN:HA	7:D:2788:EDO:H11	1.74	0.69
2:D:501:LEU:HD21	7:D:2786:EDO:H11	1.74	0.68
2:D:491:THR:HG21	7:D:2784:EDO:H11	1.78	0.66
2:D:381:GLU:HG3	9:D:3524:HOH:O	1.93	0.66
2:B:477:ARG:HD3	7:D:2784:EDO:H22	1.79	0.63
7:D:2786:EDO:C1	9:D:3010:HOH:O	2.50	0.60
2:D:311:GLU:HG2	9:D:3510:HOH:O	2.03	0.58
1:A:18:VAL:HG11	1:A:405:TYR:CE2	2.38	0.58
2:B:222:LEU:HB2	2:B:249:LEU:CD2	2.32	0.58
2:D:434:GLN:HE22	2:D:458:PHE:HA	1.71	0.56
7:D:2786:EDO:H12	9:D:3010:HOH:O	2.06	0.55
1:A:428:ILE:HG13	2:B:108:PRO:HB3	1.88	0.55
2:B:84:LEU:HD13	2:B:267[B]:MET:CE	2.33	0.54
2:B:110:ALA:HB1	2:B:267[B]:MET:HE3	1.90	0.53
1:C:347:ARG:HG3	1:C:465:LEU:HD21	1.90	0.52
2:B:381[B]:GLU:HG3	9:B:3439:HOH:O	2.09	0.52
1:A:133:LEU:HD23	1:A:133:LEU:C	2.35	0.51
1:A:84:PRO:HB2	6:A:505:CLF:S2B	2.50	0.51
2:D:359:HIS:HE1	2:D:411:TYR:OH	1.94	0.50
2:B:397:ARG:NH1	9:B:3246:HOH:O	2.44	0.50
1:C:217:THR:HG22	1:C:219:TYR:H	1.77	0.49
2:B:448:GLN:HG2	9:B:3665:HOH:O	2.12	0.49
2:B:359:HIS:HE1	2:B:411:TYR:OH	1.96	0.49
2:D:68:CYS:HB2	2:D:186:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HB3	1:A:46:ILE:HG12	1.95	0.48
2:B:267[B]:MET:HE2	2:B:268:TYR:CE1	2.49	0.47
1:C:345:GLU:HG2	9:C:1907:HOH:O	2.15	0.47
2:D:140:TYR:CD1	2:D:267[B]:MET:HE1	2.50	0.46
1:A:237:ARG:HD2	1:A:250:GLN:OE1	2.15	0.46
7:B:2782:EDO:H12	9:B:3538:HOH:O	2.15	0.46
1:C:428:ILE:HG13	2:D:108:PRO:HB3	1.98	0.46
1:C:332:GLN:HG3	9:D:3536:HOH:O	2.15	0.46
1:A:332:GLN:HG3	9:B:3643:HOH:O	2.15	0.45
1:A:55:VAL:O	1:A:403:SER:HB2	2.16	0.45
1:C:435:PRO:HA	1:C:470:TRP:CZ2	2.52	0.45
2:D:22:LEU:C	2:D:22:LEU:HD23	2.41	0.45
9:A:3122:HOH:O	2:D:359:HIS:HB2	2.17	0.45
2:D:434:GLN:NE2	2:D:458:PHE:HA	2.32	0.45
2:D:140:TYR:CG	2:D:267[B]:MET:HE1	2.52	0.45
2:B:68:CYS:HB2	2:B:186:SER:HB2	1.98	0.44
1:A:228:ASN:HA	1:A:233:ALA:H	1.83	0.44
2:B:288:LEU:HD11	2:B:298:LYS:HA	2.00	0.44
1:A:46:ILE:HD12	1:A:49:ARG:HG3	1.99	0.44
1:A:435:PRO:HA	1:A:470:TRP:CZ2	2.53	0.43
4:A:501:HCA:O2	4:A:501:HCA:O7	2.36	0.43
9:C:1882:HOH:O	2:D:117:THR:HG22	2.17	0.43
1:A:263:THR:N	1:A:264:PRO:CD	2.81	0.43
2:B:110:ALA:CB	2:B:267[B]:MET:HE3	2.49	0.43
2:B:359:HIS:CE1	2:B:411:TYR:OH	2.71	0.43
2:D:280:ALA:N	2:D:281:PRO:CD	2.81	0.43
1:C:99:TYR:HE2	9:C:1725:HOH:O	2.02	0.43
1:A:1:THR:OG1	1:A:5:GLY:HA3	2.19	0.43
1:A:72:GLY:N	1:A:73:PRO:CD	2.82	0.43
1:C:251:TRP:HA	1:C:252:SER:HA	1.76	0.42
1:C:217:THR:HB	1:C:220:ASP:OD1	2.19	0.42
1:C:332:GLN:NE2	9:C:1770:HOH:O	2.53	0.42
2:D:68:CYS:HB2	2:D:186:SER:CB	2.49	0.42
2:B:120:ALA:HB3	2:B:152:MET:HE2	2.01	0.41
2:D:9:SER:O	2:D:10:CYS:C	2.62	0.41
1:A:347:ARG:HG3	1:A:417:ASP:CG	2.45	0.41
1:A:347:ARG:NH2	9:A:3445:HOH:O	2.50	0.41
2:B:149:THR:HG23	2:B:160:LEU:HD11	2.02	0.41
2:D:366:TYR:HA	2:D:390:LEU:O	2.20	0.41
2:B:474:HIS:O	7:D:2784:EDO:H12	2.21	0.41
1:A:16:LEU:HD22	1:A:19:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:THR:N	1:C:264:PRO:CD	2.84	0.41
2:D:449:ARG:HH11	2:D:449:ARG:HD3	1.64	0.41
1:A:15:VAL:O	1:A:18:VAL:HG12	2.21	0.40
1:A:446:GLY:HA2	1:A:447:PRO:C	2.46	0.40
1:A:228:ASN:HB2	1:A:253:GLY:HA3	2.04	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%)	465 (97%)	15 (3%)	0	100	100
1	C	480/478 (100%)	463 (96%)	17 (4%)	0	100	100
2	B	527/519 (102%)	514 (98%)	11 (2%)	2 (0%)	30	14
2	D	520/519 (100%)	512 (98%)	7 (1%)	1 (0%)	43	24
All	All	2007/1994 (101%)	1954 (97%)	50 (2%)	3 (0%)	43	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	251	SER
2	B	251	SER
2	B	10	CYS

5.3.2 Protein sidechains [i](#)

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	378/397 (95%)	375 (99%)	3 (1%)	73	59
1	C	379/397 (96%)	374 (99%)	5 (1%)	61	40
2	B	432/442 (98%)	427 (99%)	5 (1%)	63	43
2	D	428/442 (97%)	425 (99%)	3 (1%)	76	63
All	All	1617/1678 (96%)	1601 (99%)	16 (1%)	70	50

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

Mol	Chain	Res	Type
1	A	97	ASN
1	A	360	HIS
1	A	443	ASP
2	B	150	THR
2	B	152	MET
2	B	267[A]	MET
2	B	267[B]	MET
2	B	397	ARG
1	C	97	ASN
1	C	217	THR
1	C	360	HIS
1	C	443	ASP
1	C	473	LEU
2	D	267[A]	MET
2	D	267[B]	MET
2	D	449	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	207	ASN
1	A	289	GLN
1	A	382	ASN
2	B	36	GLN
2	B	39	GLN
2	B	82	ASN
2	B	91	GLN
2	B	130	ASN

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Mol	Chain	Res	Type
2	B	264	HIS
2	B	290	GLN
2	B	359	HIS
2	B	478	GLN
2	B	488	ASN
1	C	112	ASN
1	C	288	HIS
2	D	91	GLN
2	D	166	ASN
2	D	274	GLN
2	D	290	GLN
2	D	359	HIS
2	D	434	GLN
2	D	478	GLN
2	D	488	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 31 ligands modelled in this entry, 9 are monoatomic - leaving 22 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
4	HCA	A	501	-	13,13,13	3.21	9 (69%)	15,18,18	2.60	5 (33%)
7	EDO	A	2776	-	3,3,3	0.45	0	2,2,2	0.20	0
7	EDO	B	2783	-	3,3,3	0.15	0	2,2,2	0.24	0
5	CFM	A	503	1	0,24,24	-	-	-	-	-
7	EDO	D	2773	-	3,3,3	0.50	0	2,2,2	0.27	0
5	CFM	C	503	1	0,24,24	-	-	-	-	-
7	EDO	A	2775	-	3,3,3	0.48	0	2,2,2	0.77	0
6	CLF	A	505	2,1	0,24,24	-	-	-	-	-
7	EDO	A	2774	-	3,3,3	0.39	0	2,2,2	0.47	0
7	EDO	D	2786	-	3,3,3	0.45	0	2,2,2	1.58	1 (50%)
6	CLF	C	505	2,1	0,24,24	-	-	-	-	-
7	EDO	D	2788	-	3,3,3	0.47	0	2,2,2	0.39	0
7	EDO	B	2778	-	3,3,3	0.63	0	2,2,2	0.59	0
7	EDO	D	2787	-	3,3,3	0.54	0	2,2,2	0.12	0
7	EDO	D	2784	-	3,3,3	0.78	0	2,2,2	2.59	1 (50%)
7	EDO	A	2777	-	3,3,3	0.56	0	2,2,2	0.55	0
7	EDO	A	2780	-	3,3,3	0.22	0	2,2,2	0.35	0
7	EDO	B	2782	-	3,3,3	0.06	0	2,2,2	0.52	0
7	EDO	B	2781	-	3,3,3	0.37	0	2,2,2	0.45	0
4	HCA	C	501	-	13,13,13	2.99	8 (61%)	15,18,18	2.84	6 (40%)
7	EDO	D	2785	-	3,3,3	0.68	0	2,2,2	0.08	0
7	EDO	C	2779	-	3,3,3	0.42	0	2,2,2	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCA	A	501	-	-	2/17/17/17	-
7	EDO	A	2776	-	-	0/1/1/1	-
7	EDO	B	2783	-	-	0/1/1/1	-
7	EDO	D	2773	-	-	1/1/1/1	-
6	CLF	A	505	2,1	-	-	0/12/10/10
7	EDO	A	2775	-	-	0/1/1/1	-
7	EDO	A	2774	-	-	0/1/1/1	-
7	EDO	D	2786	-	-	1/1/1/1	-
6	CLF	C	505	2,1	-	-	0/12/10/10
7	EDO	D	2788	-	-	1/1/1/1	-
7	EDO	B	2778	-	-	1/1/1/1	-
7	EDO	D	2787	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	D	2784	-	-	1/1/1/1	-
7	EDO	A	2777	-	-	1/1/1/1	-
7	EDO	A	2780	-	-	0/1/1/1	-
7	EDO	B	2782	-	-	0/1/1/1	-
7	EDO	B	2781	-	-	1/1/1/1	-
4	HCA	C	501	-	-	1/17/17/17	-
7	EDO	D	2785	-	-	0/1/1/1	-
7	EDO	C	2779	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	HCA	C2-C3	-5.82	1.46	1.54
4	C	501	HCA	C2-C3	-5.49	1.47	1.54
4	A	501	HCA	O7-C3	5.31	1.53	1.43
4	C	501	HCA	C2-C1	4.71	1.65	1.50
4	C	501	HCA	O7-C3	4.53	1.51	1.43
4	A	501	HCA	C3-C7	4.45	1.58	1.53
4	A	501	HCA	C2-C1	4.32	1.63	1.50
4	C	501	HCA	O6-C7	-3.55	1.17	1.30
4	A	501	HCA	O6-C7	-2.88	1.20	1.30
4	A	501	HCA	O5-C7	2.85	1.31	1.22
4	C	501	HCA	O5-C7	2.56	1.30	1.22
4	C	501	HCA	C3-C7	2.49	1.56	1.53
4	C	501	HCA	O3-C6	2.44	1.30	1.22
4	A	501	HCA	O3-C6	2.33	1.29	1.22
4	A	501	HCA	O4-C6	-2.26	1.23	1.30
4	C	501	HCA	O4-C6	-2.16	1.23	1.30
4	A	501	HCA	O1-C1	-2.02	1.15	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	HCA	O7-C3-C4	-7.77	96.45	108.88
4	A	501	HCA	O7-C3-C4	-6.66	98.24	108.88
4	C	501	HCA	O2-C1-O1	4.69	135.38	123.33
4	A	501	HCA	O2-C1-O1	4.11	133.89	123.33
4	A	501	HCA	O7-C3-C7	-3.58	103.88	108.96
7	D	2784	EDO	O1-C1-C2	3.12	136.18	112.39
4	C	501	HCA	O6-C7-C3	3.02	118.93	113.14
4	A	501	HCA	C4-C5-C6	2.68	118.98	112.77
4	A	501	HCA	O1-C1-C2	-2.56	115.71	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	HCA	O1-C1-C2	-2.47	115.94	122.95
4	C	501	HCA	O3-C6-C5	-2.36	115.60	123.09
4	C	501	HCA	O7-C3-C7	-2.35	105.62	108.96
7	D	2786	EDO	O2-C2-C1	-2.22	95.47	112.39

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	2788	EDO	O1-C1-C2-O2
7	D	2786	EDO	O1-C1-C2-O2
4	A	501	HCA	C7-C3-C4-C5
7	B	2781	EDO	O1-C1-C2-O2
7	D	2773	EDO	O1-C1-C2-O2
7	D	2784	EDO	O1-C1-C2-O2
7	A	2777	EDO	O1-C1-C2-O2
7	B	2778	EDO	O1-C1-C2-O2
4	A	501	HCA	O1-C1-C2-C3
4	C	501	HCA	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	HCA	1	0
6	A	505	CLF	1	0
7	D	2786	EDO	3	0
7	D	2788	EDO	3	0
7	D	2784	EDO	4	0
7	B	2782	EDO	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	478/478 (100%)	-0.36	3 (0%) 85 88	8, 15, 26, 35	4 (0%)
1	C	478/478 (100%)	-0.20	2 (0%) 88 91	9, 17, 27, 35	4 (0%)
2	B	519/519 (100%)	-0.50	5 (0%) 79 83	8, 13, 25, 35	10 (1%)
2	D	519/519 (100%)	-0.58	4 (0%) 82 86	8, 12, 23, 36	3 (0%)
All	All	1994/1994 (100%)	-0.41	14 (0%) 84 87	8, 14, 26, 36	21 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	120	ALA	3.4
2	D	4	ILE	3.2
2	B	122	VAL	3.1
2	D	5	ASP	2.8
1	A	22	THR	2.7
1	A	46	ILE	2.5
1	C	46	ILE	2.4
1	A	38	MET	2.3
1	C	211	GLY	2.2
2	B	121	ALA	2.2
2	B	118	GLU	2.2
2	D	126	ASN	2.1
2	D	122	VAL	2.1
2	B	4	ILE	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	D	2788	4/4	0.52	0.32	51,51,52,53	0
7	EDO	D	2786	4/4	0.86	0.20	16,27,31,31	0
7	EDO	A	2775	4/4	0.86	0.21	30,31,34,35	0
7	EDO	D	2773	4/4	0.88	0.14	20,20,21,26	0
7	EDO	A	2776	4/4	0.88	0.10	28,29,30,31	0
7	EDO	A	2780	4/4	0.88	0.15	23,30,31,32	0
7	EDO	B	2778	4/4	0.89	0.13	19,21,21,27	0
3	MG	D	3007	1/1	0.89	0.11	25,25,25,25	0
7	EDO	A	2777	4/4	0.91	0.09	26,28,28,34	0
7	EDO	D	2784	4/4	0.92	0.15	17,20,22,29	0
7	EDO	B	2782	4/4	0.93	0.09	22,22,26,35	0
7	EDO	B	2781	4/4	0.94	0.09	20,21,22,23	0
7	EDO	B	2783	4/4	0.94	0.09	17,25,28,29	0
7	EDO	D	2787	4/4	0.95	0.09	16,26,30,31	0
7	EDO	C	2779	4/4	0.95	0.07	22,24,25,25	0
7	EDO	A	2774	4/4	0.96	0.08	17,18,21,22	0
3	MG	C	3005	1/1	0.96	0.05	16,16,16,16	0
7	EDO	D	2785	4/4	0.96	0.06	15,17,18,20	0
3	MG	B	3004	1/1	0.97	0.09	19,19,19,19	0
4	HCA	C	501	14/14	0.97	0.05	8,10,14,14	0
3	MG	B	3003	1/1	0.97	0.07	20,20,20,20	0
4	HCA	A	501	14/14	0.98	0.04	8,10,13,14	0
3	MG	A	3001	1/1	0.98	0.07	17,17,17,17	0
6	CLF	A	505	15/15	0.99	0.03	8,11,13,13	0
6	CLF	C	505	15/15	0.99	0.03	7,10,12,12	0
3	MG	D	3006	1/1	0.99	0.06	10,10,10,10	0
3	MG	B	3002	1/1	0.99	0.02	9,9,9,9	0
5	CFM	A	503	17/17	0.99	0.03	8,10,10,11	0
5	CFM	C	503	17/17	0.99	0.03	10,11,12,13	0
8	CL	B	2772	1/1	0.99	0.06	16,16,16,16	0
8	CL	D	2771	1/1	1.00	0.02	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.