



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:43 PM EDT

PDB ID : 1QH1 / pdb_00001qh1
Title : NITROGENASE MOFE PROTEIN FROM KLEBSIELLA PNEUMONIAE,
PHENOSAFRANIN OXIDIZED STATE
Authors : Mayer, S.M.; Lawson, D.M.; Gormal, C.A.; Roe, S.M.; Smith, B.E.
Deposited on : 1999-05-10
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

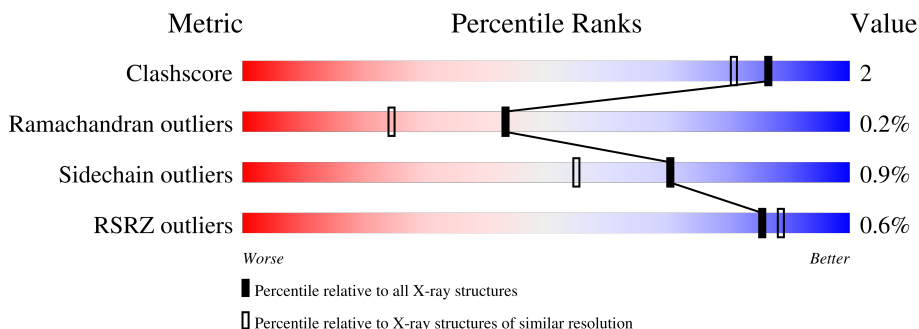
1 Overall quality at a glance

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% 13% .
1	C	478	% 87% 12% .
2	B	519	% 88% 11% .
2	D	519	% 91% 8%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18303 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	3	0
			3698	2355	630	690	23			
1	C	478	Total	C	N	O	S	0	1	0
			3706	2360	635	687	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
			4067	2601	675	760	31			
2	D	519	Total	C	N	O	S	0	3	0
			4057	2588	678	762	29			

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

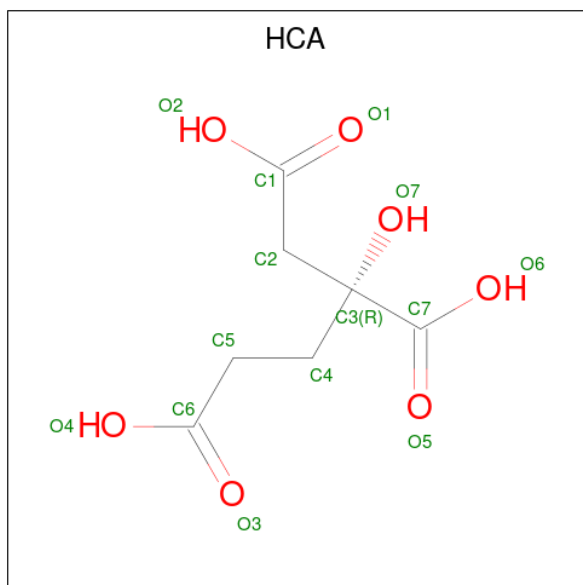
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	3	Total	Mg	0	0
			3	3		
3	C	1	Total	Mg	0	0
			1	1		

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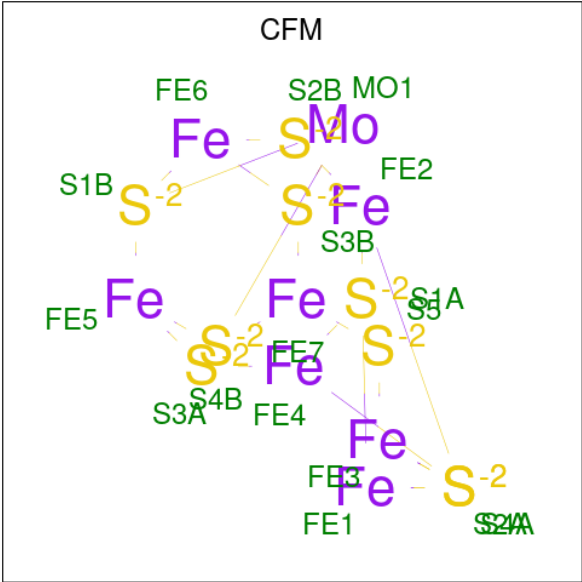
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		

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



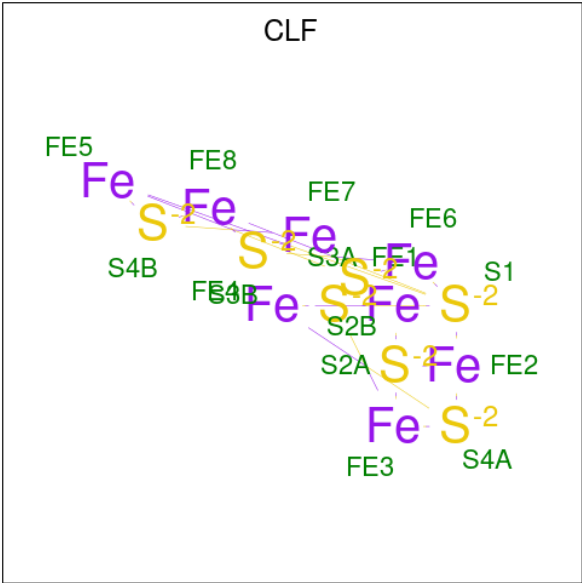
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		

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



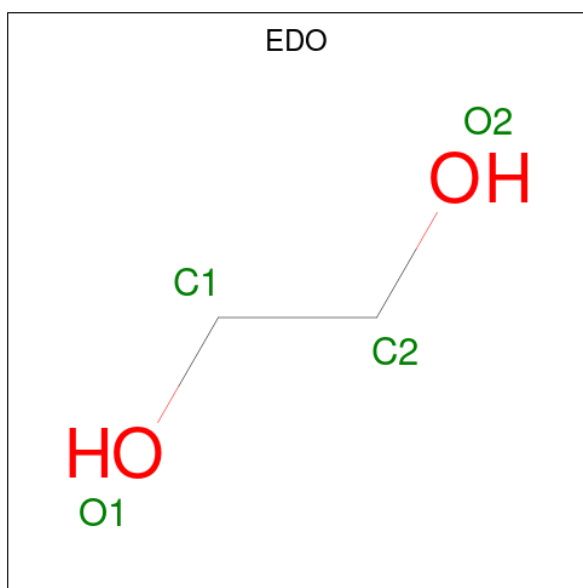
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- 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	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	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		
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 1	Cl 1	0	0
8	D	1	Total 1	Cl 1	0	0

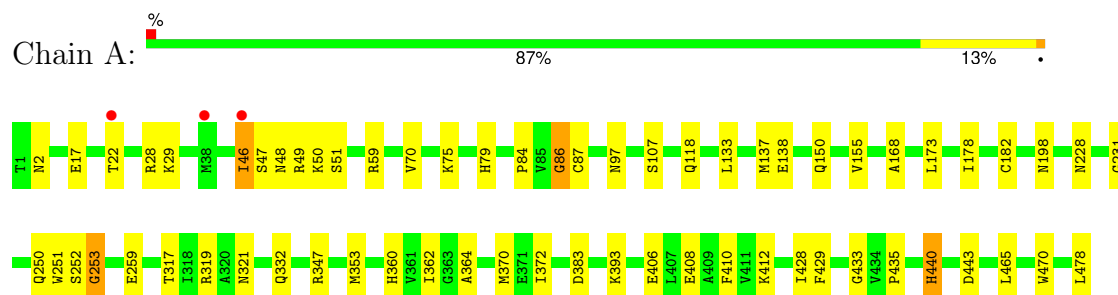
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	589	Total 589	O 589	0	0
9	B	737	Total 737	O 737	0	0
9	C	538	Total 538	O 538	0	0
9	D	758	Total 758	O 758	0	0

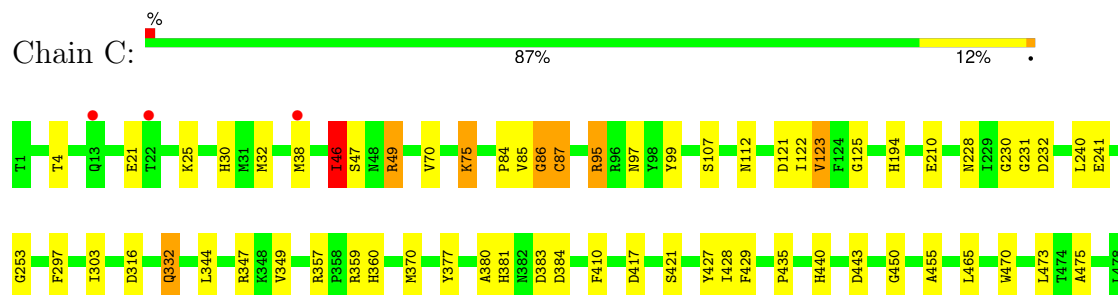
3 Residue-property plots

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.

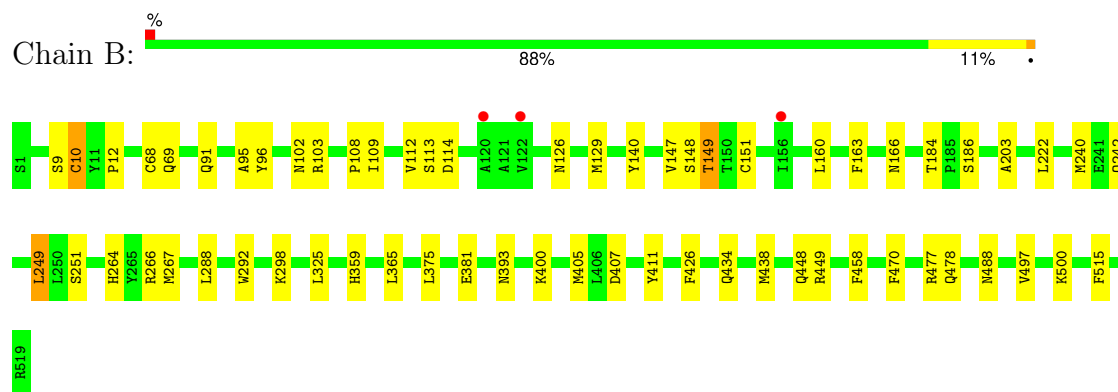
- Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



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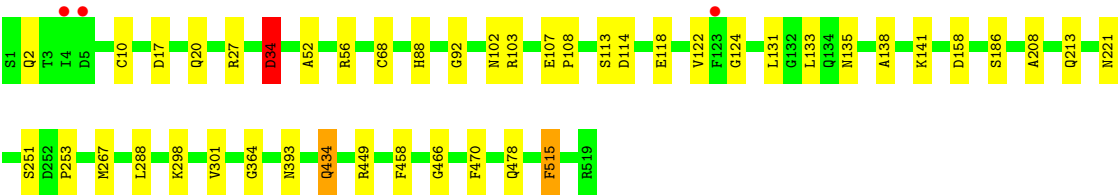


- Molecule 2: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



- 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	204.18Å 75.22Å 162.84Å 90.00° 122.88° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 50.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-1.60) 98.6 (50.00-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.199 0.154 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18303	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: CFM, MG, CLF, HCA, CL, 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	0.93	0/3795	1.59	37/5142 (0.7%)
1	C	0.91	0/3795	1.65	48/5138 (0.9%)
2	B	0.95	1/4210 (0.0%)	1.59	43/5714 (0.8%)
2	D	0.95	1/4166 (0.0%)	1.56	41/5653 (0.7%)
All	All	0.94	2/15966 (0.0%)	1.60	169/21647 (0.8%)

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	6
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	88	HIS	CD2-NE2	5.43	1.43	1.37
2	B	109	ILE	CA-C	5.04	1.58	1.52

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	449	ARG	CD-NE-CZ	13.51	143.31	124.40
2	D	434	GLN	OE1-CD-NE2	13.36	135.96	122.60
2	B	69	GLN	OE1-CD-NE2	10.04	132.64	122.60
2	D	27	ARG	CD-NE-CZ	9.70	137.98	124.40
1	C	332	GLN	OE1-CD-NE2	-9.27	113.33	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	ASP	CA-CB-CG	9.18	121.78	112.60
1	A	178	ILE	N-CA-C	9.04	117.27	107.60
1	C	122	ILE	CA-C-O	-8.76	111.56	120.85
1	A	2	ASN	OD1-CG-ND2	8.68	131.28	122.60
2	D	434	GLN	CG-CD-OE1	-8.35	104.10	120.80
2	D	434	GLN	CA-CB-CG	-8.32	97.45	114.10
1	A	50	LYS	CA-C-N	-8.11	107.94	121.39
1	A	50	LYS	C-N-CA	-8.11	107.94	121.39
1	C	241	GLU	CB-CG-CD	7.99	126.19	112.60
1	A	86	GLY	O-C-N	-7.86	112.48	122.70
2	B	405	MET	O-C-N	-7.44	114.41	122.07
2	D	213	GLN	O-C-N	7.44	127.61	121.44
2	D	470	PHE	CA-CB-CG	7.43	121.23	113.80
2	D	478	GLN	CG-CD-NE2	-7.39	105.31	116.40
2	D	114	ASP	CA-CB-CG	7.34	119.94	112.60
2	B	515	PHE	CA-CB-CG	7.32	121.12	113.80
2	D	124	GLY	N-CA-C	-7.29	103.50	112.68
1	A	383	ASP	CA-CB-CG	7.23	119.83	112.60
1	C	359	ARG	NE-CZ-NH2	7.22	125.70	119.20
1	A	332	GLN	OE1-CD-NE2	-7.20	115.40	122.60
1	C	421	SER	CA-C-O	-7.16	115.04	120.19
2	D	107	GLU	O-C-N	6.98	126.18	121.71
2	B	166	ASN	CA-CB-CG	6.94	119.54	112.60
2	B	407	ASP	CB-CG-OD2	6.91	134.29	118.40
1	A	353	MET	CA-CB-CG	6.89	127.88	114.10
2	B	393	ASN	CA-CB-CG	6.87	119.47	112.60
1	A	250	GLN	CG-CD-NE2	6.82	126.63	116.40
1	C	46	ILE	CA-C-O	-6.81	113.38	121.28
1	C	86	GLY	O-C-N	-6.79	113.88	122.70
2	D	449	ARG	CD-NE-CZ	6.78	133.89	124.40
1	C	49	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	C	122	ILE	O-C-N	6.70	128.73	121.83
1	C	429	PHE	CA-CB-CG	-6.67	107.13	113.80
1	C	359	ARG	CD-NE-CZ	6.57	133.59	124.40
2	D	221	ASN	OD1-CG-ND2	6.54	129.14	122.60
2	B	113	SER	CA-C-N	-6.48	112.36	122.67
2	B	113	SER	C-N-CA	-6.48	112.36	122.67
2	B	163	PHE	CA-CB-CG	6.42	120.22	113.80
2	B	102	ASN	CA-CB-CG	6.40	119.00	112.60
1	C	303	ILE	CA-C-O	-6.31	114.39	120.95
1	C	85	VAL	N-CA-C	6.29	120.85	112.04
1	C	70	VAL	N-CA-C	6.28	116.91	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	ARG	NE-CZ-NH2	-6.27	113.55	119.20
2	D	113	SER	CA-C-N	-6.23	112.88	122.60
2	D	113	SER	C-N-CA	-6.23	112.88	122.60
1	C	46	ILE	O-C-N	6.17	129.60	123.00
2	B	242	GLN	OE1-CD-NE2	6.10	128.70	122.60
1	A	178	ILE	N-CA-CB	-6.10	103.29	111.40
2	B	470	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	47	SER	O-C-N	-6.06	116.51	122.99
1	A	478	LEU	CA-C-O	-6.04	110.53	120.80
1	C	75	LYS	N-CA-C	6.04	118.83	111.82
2	D	478	GLN	CG-CD-OE1	6.02	132.84	120.80
1	A	79	HIS	CA-CB-CG	-6.00	107.80	113.80
1	A	317	THR	CA-CB-OG1	-6.00	100.61	109.60
2	D	17	ASP	CA-C-O	-5.94	114.59	120.82
1	A	118	GLN	CA-C-O	-5.92	114.44	121.60
2	D	107	GLU	CA-C-O	-5.92	115.05	120.50
2	D	208	ALA	CA-C-O	-5.92	114.28	120.55
1	C	230	GLY	O-C-N	5.91	129.04	122.31
1	C	410	PHE	CA-CB-CG	5.90	119.70	113.80
2	B	151	CYS	N-CA-CB	5.88	119.28	110.22
1	A	440	HIS	CA-CB-CG	5.87	119.67	113.80
1	C	377	TYR	CA-CB-CG	5.85	124.42	113.90
2	B	325	LEU	CA-C-O	-5.84	113.25	119.97
1	A	198	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	C	25	LYS	CA-C-O	-5.81	114.26	120.42
1	C	125	GLY	O-C-N	5.80	127.86	122.47
1	A	259	GLU	CB-CG-CD	-5.76	102.81	112.60
2	B	96	TYR	CA-C-O	-5.76	114.31	120.42
2	B	112	VAL	O-C-N	-5.71	116.86	122.97
2	D	102	ASN	CA-CB-CG	5.68	118.28	112.60
1	A	150	GLN	OE1-CD-NE2	5.68	128.28	122.60
2	D	133	LEU	CA-C-O	5.65	126.54	120.55
2	D	301	VAL	O-C-N	5.65	127.35	121.87
1	C	357	ARG	N-CA-C	5.64	121.36	113.57
1	C	194	HIS	O-C-N	5.64	127.88	122.07
2	D	466	GLY	CA-C-O	5.62	125.62	120.79
1	A	364	ALA	CA-C-O	-5.61	114.60	120.55
2	B	292	TRP	CA-C-O	-5.61	113.52	119.97
2	B	103	ARG	CA-C-O	-5.59	112.38	119.31
1	A	319	ARG	CD-NE-CZ	5.58	132.22	124.40
1	C	30	HIS	O-C-N	-5.58	115.22	122.37
2	B	129	MET	O-C-N	-5.58	116.21	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	GLN	CB-CA-C	-5.57	100.91	110.16
1	C	303	ILE	O-C-N	5.57	127.27	121.87
2	B	478	GLN	CG-CD-OE1	5.56	131.92	120.80
1	A	406	GLU	CA-C-O	-5.55	114.98	120.70
2	B	434	GLN	OE1-CD-NE2	5.54	128.13	122.60
2	B	264	HIS	CA-CB-CG	-5.53	108.27	113.80
2	D	103	ARG	NE-CZ-NH2	-5.52	114.23	119.20
2	D	458	PHE	CA-CB-CG	-5.49	108.31	113.80
2	B	405	MET	CA-C-O	5.49	126.58	120.82
1	A	137	MET	CA-C-O	5.48	126.57	120.82
2	B	203	ALA	CA-C-O	-5.48	114.74	120.55
1	C	112	ASN	OD1-CG-ND2	-5.48	117.12	122.60
2	D	135	ASN	O-C-N	5.47	128.38	122.15
2	D	515	PHE	CA-CB-CG	5.47	119.27	113.80
2	D	92	GLY	O-C-N	5.46	127.43	122.19
2	D	158	ASP	CA-CB-CG	5.45	118.05	112.60
2	B	488	ASN	OD1-CG-ND2	-5.43	117.17	122.60
2	D	92	GLY	CA-C-O	-5.42	115.17	120.75
1	A	168	ALA	CA-C-O	5.41	126.16	120.42
2	D	434	GLN	N-CA-C	5.41	121.77	109.81
2	B	148	SER	CA-C-O	-5.40	115.22	121.49
2	D	34	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	70	VAL	N-CA-C	5.39	116.05	110.82
2	B	147	VAL	N-CA-C	5.38	116.32	108.58
1	A	46	ILE	CA-C-O	-5.37	116.03	121.67
1	C	349	VAL	O-C-N	-5.37	117.35	123.10
1	C	417	ASP	CA-CB-CG	-5.37	107.23	112.60
1	A	410	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	48	ASN	CA-CB-CG	5.36	117.96	112.60
2	B	109	ILE	O-C-N	5.35	128.54	123.03
2	D	364	GLY	N-CA-C	-5.35	101.24	112.04
1	A	59	ARG	CD-NE-CZ	-5.34	116.93	124.40
2	B	203	ALA	O-C-N	5.33	127.77	122.12
2	D	131	LEU	O-C-N	5.33	128.23	122.15
2	B	478	GLN	CG-CD-NE2	-5.33	108.41	116.40
2	D	135	ASN	CA-C-N	-5.33	112.73	120.29
2	D	135	ASN	C-N-CA	-5.33	112.73	120.29
1	C	4	THR	CA-C-N	5.32	125.98	120.03
1	C	4	THR	C-N-CA	5.32	125.98	120.03
1	C	47	SER	O-C-N	-5.32	116.70	122.92
1	A	49	ARG	CD-NE-CZ	-5.31	116.97	124.40
2	D	20	GLN	OE1-CD-NE2	-5.31	117.29	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	477	ARG	CD-NE-CZ	-5.30	116.97	124.40
2	B	114	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	155	VAL	N-CA-C	5.30	115.50	110.42
2	B	249	LEU	CA-C-O	-5.27	114.86	120.92
1	C	440	HIS	CA-CB-CG	5.25	119.05	113.80
1	C	381	HIS	CA-CB-CG	5.25	119.05	113.80
2	D	2	GLN	CA-C-O	-5.24	114.99	121.06
2	B	488	ASN	CB-CG-ND2	5.23	124.25	116.40
1	C	450	GLY	O-C-N	-5.23	117.80	122.77
1	A	253	GLY	O-C-N	-5.23	118.91	122.62
1	C	95	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	C	316	ASP	CA-CB-CG	-5.20	107.40	112.60
2	D	52	ALA	CA-C-O	-5.20	115.03	120.55
2	D	138	ALA	N-CA-C	5.19	116.62	111.07
2	B	497	VAL	CA-C-O	5.18	126.66	121.27
2	D	141	LYS	N-CA-CB	-5.17	105.92	111.66
1	A	433	GLY	O-C-N	5.16	128.72	122.32
1	C	297	PHE	CA-CB-CG	5.16	118.96	113.80
2	D	393	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	C	87	CYS	N-CA-CB	5.15	117.62	109.94
2	B	266	ARG	NE-CZ-NH2	5.14	123.83	119.20
2	B	184	THR	O-C-N	-5.14	116.76	121.34
1	C	121	ASP	CA-CB-CG	-5.11	107.49	112.60
1	C	21	GLU	CA-C-N	5.10	127.08	120.44
1	C	21	GLU	C-N-CA	5.10	127.08	120.44
2	B	458	PHE	CA-CB-CG	-5.10	108.70	113.80
2	B	240	MET	CA-C-O	-5.07	114.37	120.10
1	A	28	ARG	CD-NE-CZ	5.07	131.50	124.40
1	A	429	PHE	CA-CB-CG	-5.05	108.75	113.80
1	C	232	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	321	ASN	CA-C-O	-5.03	115.09	120.42
2	B	149	THR	N-CA-C	5.02	117.43	109.50
1	C	475	ALA	CA-C-N	5.02	124.63	119.56
1	C	475	ALA	C-N-CA	5.02	124.63	119.56
2	B	95	ALA	O-C-N	5.01	127.44	122.12
1	C	86	GLY	CA-C-N	5.01	127.31	120.54
1	C	86	GLY	C-N-CA	5.01	127.31	120.54
1	C	344	LEU	CA-C-O	5.01	124.26	118.55

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	GLU	Mainchain
1	A	182	CYS	Mainchain
1	A	231	GLY	Mainchain
1	C	123	VAL	Mainchain
1	C	231	GLY	Mainchain
1	C	240	LEU	Mainchain
1	C	427	TYR	Mainchain
1	C	46	ILE	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	3698	0	3554	17	0
1	C	3706	0	3581	18	0
2	B	4067	0	3912	21	0
2	D	4057	0	3919	9	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	2	0
4	C	14	0	6	1	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	1	0
7	A	16	0	24	0	0
7	B	12	0	18	0	0
7	C	4	0	6	0	0
7	D	20	0	30	3	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	589	0	0	1	0
9	B	737	0	0	6	0
9	C	538	0	0	5	0
9	D	758	0	0	2	0
All	All	18303	0	15056	65	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 (65) 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	1.68	0.76
1:C:347:ARG:HG3	1:C:465:LEU:HD21	1.69	0.75
1:C:210:GLU:OE2	1:C:210:GLU:CG	2.37	0.73
1:A:428:ILE:HG13	2:B:108:PRO:HB3	1.79	0.65
1:A:408:GLU:HG2	1:A:412:LYS:HE3	1.79	0.65
2:D:515:PHE:CE1	7:D:2780:EDO:H22	2.36	0.61
2:B:365[A]:LEU:HD13	2:B:375:LEU:HD23	1.83	0.60
2:D:515:PHE:HE1	7:D:2780:EDO:H22	1.66	0.60
4:A:501:HCA:O2	4:A:501:HCA:O7	2.19	0.59
1:A:347:ARG:HG3	1:A:465:LEU:HD21	1.85	0.57
1:A:84:PRO:HB2	6:A:505:CLF:S2B	2.46	0.56
2:B:68:CYS:HB2	2:B:186:SER:HB2	1.88	0.55
2:B:140:TYR:HD1	2:B:267[B]:MET:HE1	1.71	0.55
1:A:347:ARG:HB2	1:A:370:MET:HE3	1.89	0.55
2:B:365[A]:LEU:CD1	2:B:375:LEU:HD23	2.38	0.53
2:B:448:GLN:HG2	9:B:3684:HOH:O	2.09	0.53
1:A:393:LYS:HE3	9:A:3556:HOH:O	2.09	0.52
2:B:400:LYS:HE2	9:B:3538:HOH:O	2.09	0.52
2:D:68:CYS:HB2	2:D:186:SER:HB2	1.91	0.51
2:B:140:TYR:CD1	2:B:267[B]:MET:HE1	2.45	0.51
1:C:332:GLN:HG3	9:C:2528:HOH:O	2.11	0.51
2:B:500:LYS:HE3	9:B:3511:HOH:O	2.10	0.50
2:B:149:THR:HG23	2:B:160:LEU:HD11	1.93	0.50
1:A:29:LYS:HB3	1:A:46:ILE:HG12	1.93	0.50
1:C:455:ALA:HB2	9:C:1763:HOH:O	2.12	0.50
4:C:501:HCA:O2	4:C:501:HCA:O7	2.30	0.49
1:C:332:GLN:NE2	9:C:1763:HOH:O	2.45	0.49
1:C:435:PRO:HA	1:C:470:TRP:CZ2	2.48	0.48
1:C:46:ILE:HD12	1:C:49:ARG:HD2	1.95	0.48
1:C:99:TYR:HE2	9:C:1653:HOH:O	1.97	0.48
9:C:1571:HOH:O	2:D:118:GLU:HG3	2.14	0.48
2:D:34:ASP:HB3	9:D:3613:HOH:O	2.13	0.48
2:B:359:HIS:CE1	2:B:411:TYR:OH	2.67	0.48
2:D:68:CYS:HB2	2:D:186:SER:CB	2.44	0.48
1:C:428:ILE:HG13	2:D:108:PRO:HB3	1.97	0.47
2:D:288:LEU:HD11	2:D:298:LYS:HA	1.96	0.47
2:B:359:HIS:HE1	2:B:411:TYR:OH	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD23	1:A:133:LEU:C	2.40	0.45
1:C:380:ALA:HB1	1:C:384:ASP:HB2	1.97	0.45
2:B:126:ASN:HB2	9:B:3278:HOH:O	2.17	0.45
2:B:288:LEU:HD11	2:B:298:LYS:HA	1.99	0.45
1:C:32:MET:HE1	1:C:38:MET:HE1	1.98	0.45
1:A:51[B]:SER:OG	2:B:91:GLN:NE2	2.37	0.45
1:C:32:MET:CE	1:C:38:MET:HE1	2.47	0.45
1:A:435:PRO:HA	1:A:470:TRP:CZ2	2.51	0.45
1:C:347:ARG:HB2	1:C:370:MET:HE3	1.99	0.45
1:A:75:LYS:O	1:A:107[B]:SER:HA	2.16	0.45
2:B:426:PHE:CE2	2:B:438[A]:MET:HE3	2.52	0.44
2:B:9:SER:O	2:B:10:CYS:C	2.61	0.44
1:A:362:ILE:HG12	1:A:372:ILE:HG13	1.99	0.44
9:B:3684:HOH:O	7:D:2780:EDO:H21	2.17	0.43
1:C:228:ASN:HB2	1:C:253:GLY:HA3	2.00	0.42
1:A:251:TRP:HA	1:A:252:SER:HA	1.79	0.42
2:B:68:CYS:HB2	2:B:186:SER:CB	2.49	0.42
1:A:86:GLY:O	1:A:87:CYS:C	2.61	0.42
2:B:381[B]:GLU:HG3	9:B:3435:HOH:O	2.19	0.42
1:A:138:GLU:HG2	1:A:173:LEU:HD22	2.01	0.41
1:C:46:ILE:HD12	1:C:49:ARG:CD	2.50	0.41
2:D:267:MET:HE2	9:D:3517:HOH:O	2.20	0.41
1:A:228:ASN:HB2	1:A:253:GLY:HA3	2.03	0.41
2:B:426:PHE:HE2	2:B:438[A]:MET:HE3	1.85	0.41
1:C:86:GLY:O	1:C:87:CYS:C	2.62	0.41
1:A:440:HIS:HB3	4:A:501:HCA:O5	2.21	0.40
1:C:75:LYS:O	1:C:107[B]:SER:HA	2.20	0.40
1:C:84:PRO:HB2	6:C:505:CLF:S2B	2.61	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	479/478 (100%)	461 (96%)	18 (4%)	0	100	100
1	C	477/478 (100%)	460 (96%)	17 (4%)	0	100	100
2	B	527/519 (102%)	516 (98%)	9 (2%)	2 (0%)	30	14
2	D	520/519 (100%)	508 (98%)	10 (2%)	2 (0%)	30	14
All	All	2003/1994 (100%)	1945 (97%)	54 (3%)	4 (0%)	43	24

All (4) Ramachandran outliers are listed below:

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

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	376/397 (95%)	372 (99%)	4 (1%)	65	46
1	C	377/397 (95%)	372 (99%)	5 (1%)	61	40
2	B	430/442 (97%)	429 (100%)	1 (0%)	87	81
2	D	429/442 (97%)	424 (99%)	5 (1%)	63	43
All	All	1612/1678 (96%)	1597 (99%)	15 (1%)	70	55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	97	ASN
1	A	360	HIS
1	A	443	ASP
2	B	12	PRO
1	C	97	ASN
1	C	123	VAL

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Mol	Chain	Res	Type
1	C	360	HIS
1	C	443	ASP
1	C	473	LEU
2	D	34	ASP
2	D	56	ARG
2	D	122	VAL
2	D	253	PRO
2	D	434	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	382	ASN
2	B	39	GLN
2	B	82	ASN
2	B	91	GLN
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	262	ASN
1	C	288	HIS
1	C	467	ASN
2	D	33	HIS
2	D	91	GLN
2	D	290	GLN
2	D	302	GLN
2	D	359	HIS
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 [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 28 ligands modelled in this entry, 9 are monoatomic - leaving 19 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	D	2785	-	3,3,3	0.42	0	2,2,2	0.18	0
7	EDO	A	2776	-	3,3,3	0.49	0	2,2,2	0.89	0
7	EDO	D	2783	-	3,3,3	0.68	0	2,2,2	0.29	0
7	EDO	D	2780	-	3,3,3	0.72	0	2,2,2	0.93	0
4	HCA	C	501	5	13,13,13	2.87	7 (53%)	15,18,18	3.08	7 (46%)
7	EDO	A	2775	-	3,3,3	0.47	0	2,2,2	0.47	0
7	EDO	C	2782	-	3,3,3	0.32	0	2,2,2	0.54	0
7	EDO	A	2774	-	3,3,3	0.43	0	2,2,2	0.56	0
7	EDO	B	2778	-	3,3,3	0.43	0	2,2,2	0.43	0
5	CFM	A	503	1,4	0,24,24	-	-	-	-	-
7	EDO	B	2781	-	3,3,3	0.57	0	2,2,2	0.18	0
5	CFM	C	503	1,4	0,24,24	-	-	-	-	-
6	CLF	C	505	2,1	0,24,24	-	-	-	-	-
7	EDO	D	2773	-	3,3,3	0.46	0	2,2,2	0.59	0
6	CLF	A	505	2,1	0,24,24	-	-	-	-	-
7	EDO	D	2784	-	3,3,3	0.73	0	2,2,2	0.19	0
4	HCA	A	501	5	13,13,13	2.92	7 (53%)	15,18,18	2.76	5 (33%)
7	EDO	B	2779	-	3,3,3	0.64	0	2,2,2	0.41	0
7	EDO	A	2777	-	3,3,3	0.32	0	2,2,2	0.56	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	C	501	5	-	1/17/17/17	-
7	EDO	A	2775	-	-	0/1/1/1	-
7	EDO	B	2781	-	-	1/1/1/1	-
7	EDO	D	2785	-	-	0/1/1/1	-
4	HCA	A	501	5	-	3/17/17/17	-
7	EDO	D	2773	-	-	1/1/1/1	-
6	CLF	C	505	2,1	-	-	0/12/10/10
7	EDO	C	2782	-	-	0/1/1/1	-
7	EDO	B	2779	-	-	0/1/1/1	-
7	EDO	A	2776	-	-	1/1/1/1	-
7	EDO	D	2783	-	-	0/1/1/1	-
6	CLF	A	505	2,1	-	-	0/12/10/10
7	EDO	A	2774	-	-	0/1/1/1	-
7	EDO	B	2778	-	-	0/1/1/1	-
7	EDO	A	2777	-	-	0/1/1/1	-
7	EDO	D	2780	-	-	1/1/1/1	-
7	EDO	D	2784	-	-	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	-5.22	1.47	1.54
4	C	501	HCA	C2-C1	5.18	1.66	1.50
4	A	501	HCA	C2-C1	4.68	1.64	1.50
4	C	501	HCA	C2-C3	-4.51	1.48	1.54
4	C	501	HCA	O7-C3	4.37	1.51	1.43
4	A	501	HCA	C3-C7	4.07	1.57	1.53
4	A	501	HCA	O7-C3	3.71	1.50	1.43
4	C	501	HCA	C3-C7	3.41	1.57	1.53
4	A	501	HCA	O6-C7	-3.22	1.18	1.30
4	C	501	HCA	O6-C7	-3.08	1.19	1.30
4	C	501	HCA	O5-C7	3.06	1.31	1.22
4	A	501	HCA	O3-C6	2.63	1.30	1.22
4	A	501	HCA	O5-C7	2.37	1.29	1.22
4	C	501	HCA	O3-C6	2.04	1.28	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	HCA	O2-C1-O1	6.60	140.30	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	HCA	O7-C3-C4	-6.53	98.43	108.88
4	C	501	HCA	O7-C3-C4	-5.74	99.71	108.88
4	A	501	HCA	O2-C1-O1	5.52	137.54	123.33
4	C	501	HCA	O1-C1-C2	-4.02	111.57	122.95
4	C	501	HCA	O6-C7-C3	3.55	119.96	113.14
4	C	501	HCA	C4-C5-C6	3.53	120.95	112.77
4	A	501	HCA	O1-C1-C2	-3.52	112.98	122.95
4	A	501	HCA	C4-C5-C6	3.04	119.81	112.77
4	C	501	HCA	O7-C3-C7	-2.89	104.86	108.96
4	A	501	HCA	O6-C7-C3	2.40	117.74	113.14
4	C	501	HCA	O3-C6-C5	-2.05	116.60	123.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	HCA	C7-C3-C4-C5
7	B	2781	EDO	O1-C1-C2-O2
7	A	2776	EDO	O1-C1-C2-O2
7	D	2773	EDO	O1-C1-C2-O2
7	D	2780	EDO	O1-C1-C2-O2
4	A	501	HCA	O1-C1-C2-C3
4	A	501	HCA	O2-C1-C2-C3
4	C	501	HCA	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	2780	EDO	3	0
4	C	501	HCA	1	0
6	C	505	CLF	1	0
6	A	505	CLF	1	0
4	A	501	HCA	2	0

5.7 Other polymers [i](#)

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 [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%)	-0.29	3 (0%) 85 88	11, 18, 30, 40	3 (0%)
1	C	478/478 (100%)	-0.23	3 (0%) 85 88	11, 20, 31, 40	1 (0%)
2	B	519/519 (100%)	-0.41	3 (0%) 85 88	8, 17, 29, 38	10 (1%)
2	D	519/519 (100%)	-0.55	3 (0%) 85 88	9, 15, 26, 38	3 (0%)
All	All	1994/1994 (100%)	-0.37	12 (0%) 85 88	8, 17, 29, 40	17 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	5	ASP	4.1
2	B	156	ILE	2.9
2	B	122	VAL	2.6
2	D	4	ILE	2.6
1	C	13	GLN	2.4
1	C	22	THR	2.3
1	C	38	MET	2.3
1	A	46	ILE	2.2
1	A	22	THR	2.2
1	A	38	MET	2.1
2	D	123	PHE	2.1
2	B	120	ALA	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 ⓘ

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	2776	4/4	0.84	0.12	30,33,36,36	0
7	EDO	A	2775	4/4	0.85	0.18	30,33,34,34	0
7	EDO	B	2781	4/4	0.90	0.12	21,21,22,25	0
7	EDO	D	2773	4/4	0.90	0.12	21,22,25,25	0
7	EDO	D	2780	4/4	0.92	0.10	24,25,26,30	0
7	EDO	A	2777	4/4	0.93	0.09	33,33,34,37	0
3	MG	B	3004	1/1	0.93	0.07	25,25,25,25	0
7	EDO	B	2778	4/4	0.94	0.09	24,24,25,26	0
7	EDO	C	2782	4/4	0.94	0.10	28,28,29,29	0
3	MG	B	3003	1/1	0.95	0.07	27,27,27,27	0
3	MG	D	3007	1/1	0.95	0.08	29,29,29,29	0
7	EDO	B	2779	4/4	0.96	0.08	17,20,22,22	0
7	EDO	D	2783	4/4	0.96	0.07	17,19,19,23	0
7	EDO	D	2784	4/4	0.96	0.07	15,18,20,20	0
7	EDO	A	2774	4/4	0.97	0.07	20,23,24,25	0
4	HCA	C	501	14/14	0.97	0.05	12,14,16,16	0
7	EDO	D	2785	4/4	0.97	0.09	19,27,27,30	0
3	MG	A	3001	1/1	0.98	0.07	18,18,18,18	0
6	CLF	A	505	15/15	0.98	0.04	12,15,17,17	0
4	HCA	A	501	14/14	0.98	0.04	11,14,16,16	0
8	CL	B	2771	1/1	0.98	0.08	20,20,20,20	0
5	CFM	A	503	17/17	0.99	0.03	11,13,14,15	0
5	CFM	C	503	17/17	0.99	0.03	12,14,15,16	0
3	MG	B	3002	1/1	0.99	0.02	12,12,12,12	0
6	CLF	C	505	15/15	0.99	0.03	11,13,14,15	0
3	MG	C	3005	1/1	0.99	0.03	19,19,19,19	0
3	MG	D	3006	1/1	0.99	0.04	12,12,12,12	0
8	CL	D	2772	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.