Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 01:25 AM EDT

PDB ID	:	1QH8
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:

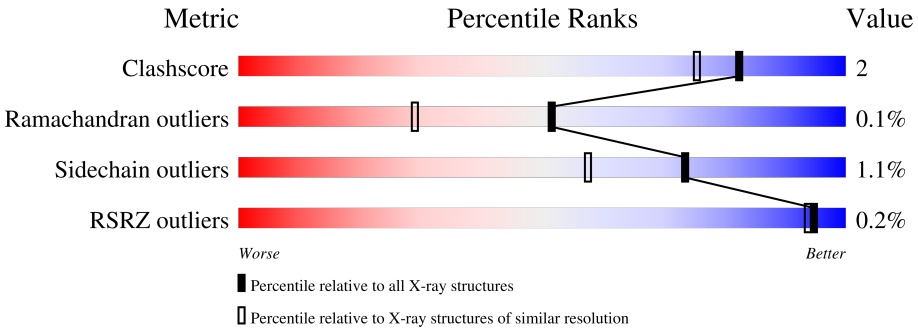
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 <=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	88% 11%
1	C	478	89% 10%
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 (i)

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 (three-letter code: 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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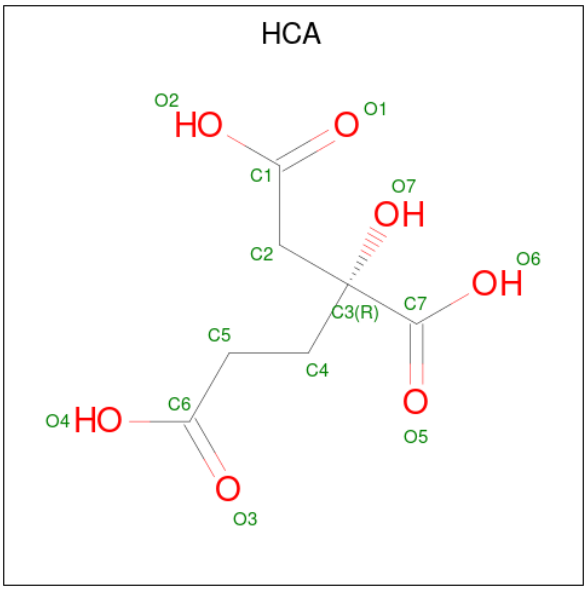
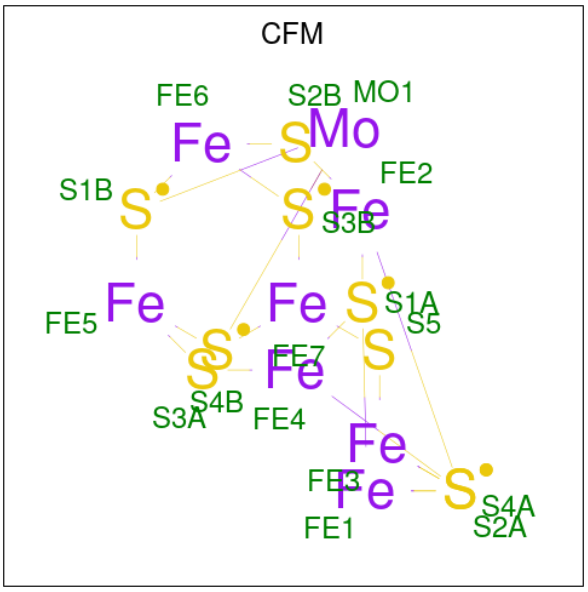
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Mg 2 2	0	0

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



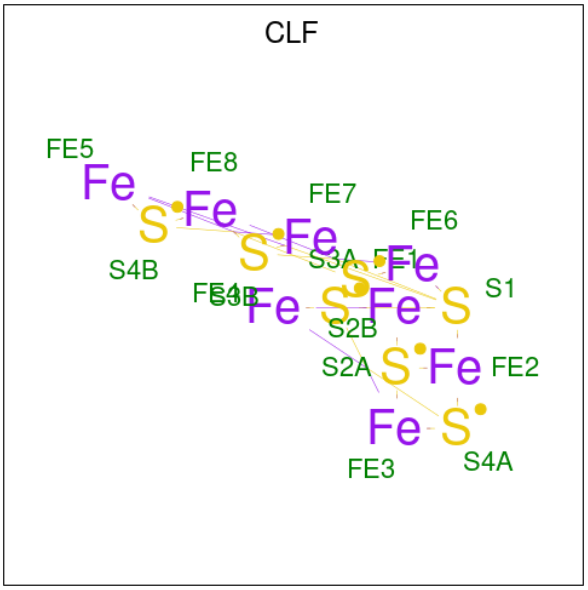
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 14 7 7	0	0
4	C	1	Total C O 14 7 7	0	0

- Molecule 5 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).



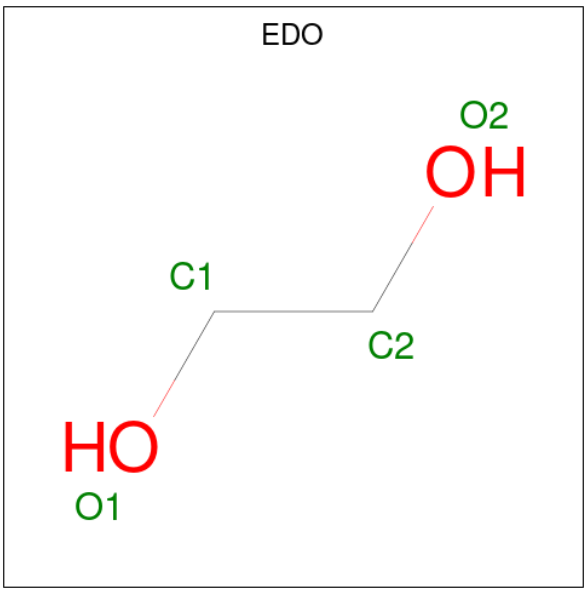
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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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 (three-letter code: 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.

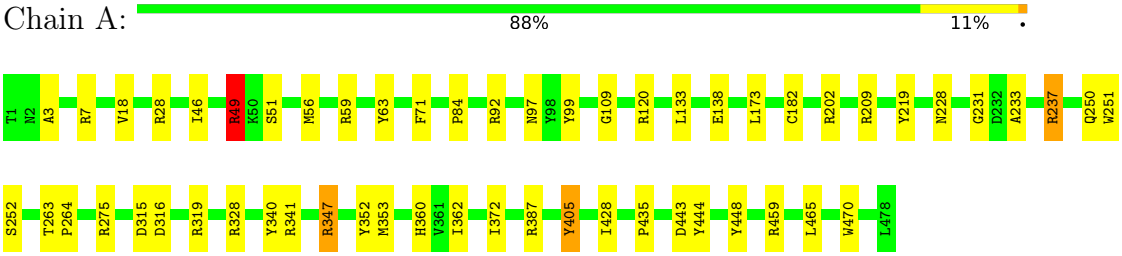
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	611	Total O 611 611	0	0
9	B	810	Total O 810 810	0	0
9	C	595	Total O 595 595	0	0
9	D	824	Total O 824 824	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

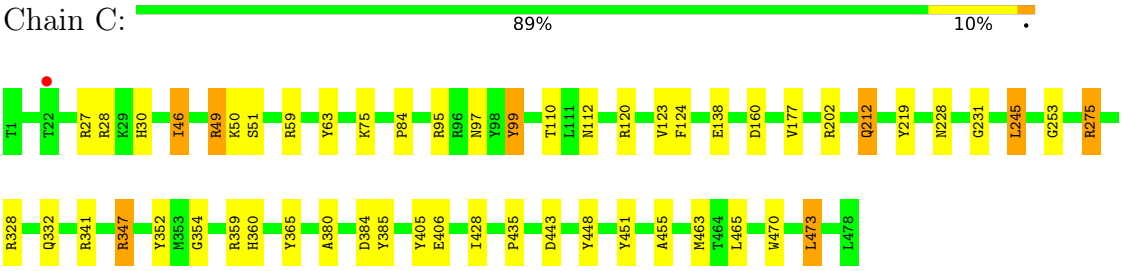
• Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)

Chain A:



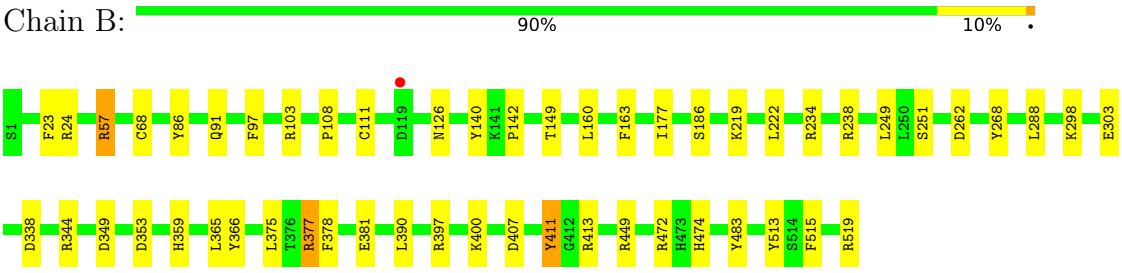
• Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)

Chain C:



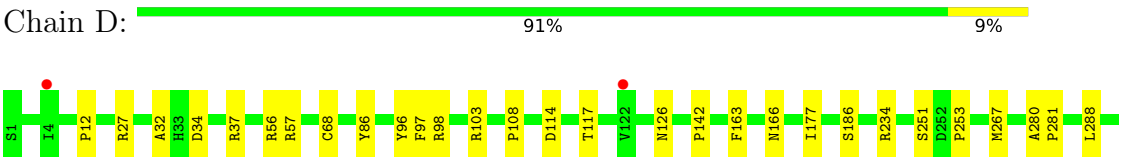
• Molecule 2: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)

Chain B:



• Molecule 2: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)

Chain D:




K298
D322
R344
D353
H359
F371
K404
Y411
R427
R433
Q434
F446
R449
R464
R472
R477
Q478
T491
D512
R519

4 Data and refinement statistics (i)

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 – 1.60 136.27 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-1.60) 97.8 (136.27-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.155 , 0.197 0.177 , (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 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, MG, HCA, CL, CFM, CLF

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	0.66	0/3815	1.37	36/5165 (0.7%)
1	C	0.66	0/3811	1.34	34/5158 (0.7%)
2	B	0.66	0/4192	1.37	36/5686 (0.6%)
2	D	0.68	0/4186	1.34	37/5679 (0.7%)
All	All	0.67	0/16004	1.35	143/21688 (0.7%)

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 (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	407	ASP	CB-CG-OD2	17.14	133.72	118.30
2	B	449	ARG	CD-NE-CZ	16.58	146.82	123.60
2	D	103	ARG	NE-CZ-NH2	-14.31	113.14	120.30
2	D	103	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	A	387	ARG	NE-CZ-NH2	-11.96	114.32	120.30
2	B	103	ARG	NE-CZ-NH2	-11.89	114.35	120.30
2	D	519	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	C	352	TYR	CB-CG-CD2	11.16	127.69	121.00
2	D	427	ARG	NE-CZ-NH2	-11.09	114.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	347	ARG	NE-CZ-NH1	10.90	125.75	120.30
2	D	449	ARG	NE-CZ-NH2	-10.57	115.01	120.30
2	D	519	ARG	NE-CZ-NH2	-10.22	115.19	120.30
2	B	472	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	C	27	ARG	NE-CZ-NH2	-9.97	115.31	120.30
2	B	103	ARG	NE-CZ-NH1	9.77	125.19	120.30
2	B	349	ASP	CB-CG-OD2	-9.64	109.62	118.30
2	B	483	TYR	CB-CG-CD2	-9.64	115.22	121.00
2	B	397	ARG	NE-CZ-NH2	-9.52	115.54	120.30
2	D	371	PHE	CB-CG-CD2	-9.38	114.23	120.80
2	B	234	ARG	NE-CZ-NH2	-9.35	115.62	120.30
2	B	411	TYR	CB-CG-CD1	-9.31	115.41	121.00
1	A	347	ARG	CD-NE-CZ	9.31	136.63	123.60
2	B	377	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	C	275	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	A	275	ARG	NE-CZ-NH2	-9.06	115.77	120.30
2	B	472	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	63	TYR	CB-CG-CD1	-8.64	115.82	121.00
2	D	353	ASP	CB-CG-OD1	8.63	126.07	118.30
2	B	234	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	448	TYR	CB-CG-CD2	-8.45	115.93	121.00
1	C	49	ARG	NE-CZ-NH2	-8.34	116.13	120.30
2	D	449	ARG	CD-NE-CZ	8.30	135.23	123.60
1	A	28	ARG	NE-CZ-NH2	-8.27	116.17	120.30
2	D	27	ARG	CD-NE-CZ	8.25	135.15	123.60
1	A	328	ARG	CD-NE-CZ	8.12	134.97	123.60
2	B	338	ASP	CB-CG-OD1	8.08	125.57	118.30
2	D	464	ARG	NE-CZ-NH2	-8.03	116.28	120.30
2	D	234	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	209	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	C	28	ARG	CD-NE-CZ	7.66	134.32	123.60
2	B	238	ARG	NE-CZ-NH1	7.62	124.11	120.30
2	B	338	ASP	CB-CG-OD2	-7.59	111.47	118.30
2	D	353	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	C	385	TYR	CB-CG-CD1	-7.57	116.46	121.00
1	A	120	ARG	CA-CB-CG	7.50	129.91	113.40
1	A	28	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	C	448	TYR	CB-CG-CD1	7.33	125.40	121.00
1	A	49	ARG	CD-NE-CZ	7.32	133.84	123.60
2	D	98	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	237	ARG	NE-CZ-NH2	-7.27	116.66	120.30
2	B	349	ASP	CB-CG-OD1	7.25	124.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	483	TYR	CB-CG-CD1	7.15	125.29	121.00
1	A	49	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	341	ARG	NE-CZ-NH2	-7.11	116.75	120.30
2	D	427	ARG	NE-CZ-NH1	7.10	123.85	120.30
2	B	519	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	319	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	202	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	C	59	ARG	NE-CZ-NH2	-6.87	116.87	120.30
2	D	163	PHE	CB-CG-CD1	6.86	125.60	120.80
1	C	341	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	B	57	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	202	ARG	NE-CZ-NH2	-6.65	116.98	120.30
2	D	37	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	328	ARG	CD-NE-CZ	6.54	132.75	123.60
1	C	359	ARG	NE-CZ-NH2	6.48	123.54	120.30
2	B	238	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	319	ARG	NE-CZ-NH2	-6.45	117.08	120.30
2	D	477	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	328	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	219	TYR	CB-CG-CD2	-6.36	117.18	121.00
2	B	353	ASP	CB-CG-OD1	6.35	124.02	118.30
2	D	86	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	C	448	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	A	405	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	C	352	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	A	319	ARG	CD-NE-CZ	6.17	132.24	123.60
1	C	347	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	D	322	ASP	CB-CG-OD1	6.13	123.82	118.30
2	B	353	ASP	CB-CG-OD2	-6.13	112.79	118.30
2	B	407	ASP	OD1-CG-OD2	-6.12	111.67	123.30
2	B	163	PHE	CB-CG-CD1	6.11	125.08	120.80
2	D	433	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	49	ARG	NE-CZ-NH2	-6.05	117.27	120.30
2	D	96	TYR	CB-CG-CD2	-5.99	117.40	121.00
1	C	359	ARG	CD-NE-CZ	5.99	131.98	123.60
2	B	268	TYR	CB-CG-CD2	-5.97	117.42	121.00
2	D	57	ARG	NE-CZ-NH2	-5.97	117.32	120.30
2	D	234	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	D	446	PHE	CB-CG-CD2	-5.94	116.64	120.80
1	A	353	MET	CA-CB-CG	5.93	123.38	113.30
1	A	387	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	352	TYR	CB-CG-CD1	-5.91	117.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	50	LYS	C-N-CA	-5.88	107.00	121.70
2	D	411	TYR	CB-CG-CD1	-5.86	117.48	121.00
2	D	322	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	C	51	SER	N-CA-CB	-5.85	101.73	110.50
1	C	451	TYR	CB-CG-CD2	-5.82	117.51	121.00
2	B	378	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	C	138	GLU	OE1-CD-OE2	-5.75	116.39	123.30
2	D	267	MET	CA-CB-CG	5.73	123.04	113.30
1	C	328	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	459	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	B	24	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	B	140	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	C	473	LEU	CA-CB-CG	5.69	128.38	115.30
1	C	359	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	C	405	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	C	99	TYR	CB-CG-CD1	-5.64	117.61	121.00
2	D	449	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	316	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	30	HIS	O-C-N	-5.60	113.75	122.70
1	A	71	PHE	CB-CG-CD2	-5.53	116.93	120.80
2	D	477	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	B	86	TYR	CB-CG-CD2	-5.45	117.73	121.00
2	D	478	GLN	CG-CD-OE1	5.42	132.44	121.60
2	B	262	ASP	CB-CG-OD1	5.42	123.17	118.30
2	B	413	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	63	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	C	365	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	C	46	ILE	O-C-N	5.31	131.20	122.70
1	A	275	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	D	97	PHE	CB-CG-CD2	-5.29	117.10	120.80
2	B	23	PHE	CB-CG-CD2	-5.28	117.10	120.80
2	B	97	PHE	CB-CG-CD2	-5.27	117.11	120.80
2	D	512	ASP	CB-CG-OD1	5.27	123.05	118.30
2	D	344	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	444	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	D	434	GLN	CA-CB-CG	-5.20	101.96	113.40
2	B	344	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	160	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	448	TYR	CB-CG-CD1	5.15	124.09	121.00
1	A	315	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	347	ARG	NE-CZ-NH1	5.09	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	406	GLU	OE1-CD-OE2	-5.08	117.21	123.30
2	D	472	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	365	TYR	CG-CD1-CE1	-5.06	117.25	121.30
1	C	405	TYR	CB-CG-CD1	5.05	124.03	121.00
2	D	114	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	340	TYR	CG-CD1-CE1	-5.01	117.29	121.30
1	A	63	TYR	CB-CG-CD2	5.00	124.00	121.00
2	B	513	TYR	CB-CG-CD1	5.00	124.00	121.00

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 (i)

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	21	0
1	C	3716	0	3593	22	0
2	B	4067	0	3926	20	0
2	D	4060	0	3918	14	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	2	0
All	All	18565	0	15118	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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
1:A:133:LEU:HD23	1:A:133:LEU:C	2.37	0.43
7:B:2907:EDO:C2	2:D:491:THR:OG1	2.66	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
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

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%)	47	26
2	D	523/519 (101%)	513 (98%)	9 (2%)	1 (0%)	47	26
All	All	2004/1994 (100%)	1950 (97%)	52 (3%)	2 (0%)	51	29

All (2) Ramachandran outliers are listed below:

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

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	380/397 (96%)	376 (99%)	4 (1%)	73	57
1	C	379/397 (96%)	372 (98%)	7 (2%)	59	36
2	B	429/442 (97%)	428 (100%)	1 (0%)	93	88
2	D	434/442 (98%)	428 (99%)	6 (1%)	67	47
All	All	1622/1678 (97%)	1604 (99%)	18 (1%)	73	57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	97	ASN
1	A	360	HIS
1	A	443	ASP
2	B	126	ASN
1	C	97	ASN
1	C	112	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	56	ARG
2	D	126	ASN
2	D	253	PRO
2	D	404	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN

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Mol	Chain	Res	Type
2	B	91	GLN
2	B	264	HIS
2	B	359	HIS
1	C	112	ASN
1	C	118	GLN
2	D	91	GLN
2	D	359	HIS
2	D	434	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

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	D	2918	-	3,3,3	0.39	0	2,2,2	0.15	0
7	EDO	C	2914	-	3,3,3	0.32	0	2,2,2	0.45	0
6	CLF	C	505[B]	1,2	0,24,24	-	-	-		
7	EDO	A	2915	-	3,3,3	0.26	0	2,2,2	0.25	0
7	EDO	B	2905	-	3,3,3	0.11	0	2,2,2	0.42	0
7	EDO	A	2910	-	3,3,3	0.53	0	2,2,2	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	D	2917	-	3,3,3	0.67	0	2,2,2	0.09	0
7	EDO	D	2919	-	3,3,3	0.36	0	2,2,2	0.39	0
7	EDO	B	2907	-	3,3,3	0.68	0	2,2,2	2.87	2 (100%)
4	HCA	C	501	-	13,13,13	2.93	6 (46%)	14,18,18	2.98	7 (50%)
7	EDO	A	2911	-	3,3,3	0.38	0	2,2,2	0.18	0
7	EDO	A	2909	-	3,3,3	0.48	0	2,2,2	0.52	0
7	EDO	D	2916	-	3,3,3	0.60	0	2,2,2	0.08	0
7	EDO	A	2912	-	3,3,3	0.34	0	2,2,2	0.39	0
6	CLF	A	505[A]	2	0,24,24	-	-	-		
5	CFM	C	503	1	0,24,24	-	-	-		
7	EDO	B	2903	-	3,3,3	0.43	0	2,2,2	0.64	0
7	EDO	B	2906	-	3,3,3	0.54	0	2,2,2	0.30	0
4	HCA	A	501	-	13,13,13	2.97	7 (53%)	14,18,18	2.48	4 (28%)
7	EDO	B	2904	-	3,3,3	0.60	0	2,2,2	1.31	0
6	CLF	C	505[A]	1,2	0,24,24	-	-	-		
7	EDO	D	2908	-	3,3,3	0.46	0	2,2,2	0.53	0
6	CLF	A	505[B]	1,2	0,24,24	-	-	-		
7	EDO	B	2913	-	3,3,3	0.48	0	2,2,2	0.23	0
5	CFM	A	503	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	D	2918	-	-	0/1/1/1	-
7	EDO	C	2914	-	-	0/1/1/1	-
6	CLF	C	505[B]	1,2	-	-	0/12/10/10
7	EDO	A	2915	-	-	0/1/1/1	-
7	EDO	B	2905	-	-	0/1/1/1	-
7	EDO	A	2910	-	-	0/1/1/1	-
7	EDO	D	2919	-	-	1/1/1/1	-
7	EDO	D	2917	-	-	0/1/1/1	-
7	EDO	B	2907	-	-	1/1/1/1	-
4	HCA	C	501	-	-	2/17/17/17	-
7	EDO	A	2911	-	-	1/1/1/1	-
7	EDO	A	2909	-	-	0/1/1/1	-
7	EDO	D	2916	-	-	0/1/1/1	-
7	EDO	A	2912	-	-	0/1/1/1	-
6	CLF	A	505[A]	2	-	-	0/12/10/10
7	EDO	B	2903	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	2906	-	-	1/1/1/1	-
4	HCA	A	501	-	-	2/17/17/17	-
7	EDO	B	2904	-	-	1/1/1/1	-
6	CLF	C	505[A]	1,2	-	-	0/12/10/10
7	EDO	D	2908	-	-	1/1/1/1	-
6	CLF	A	505[B]	1,2	-	-	0/12/10/10
7	EDO	B	2913	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	HCA	C2-C3	-5.49	1.47	1.53
4	C	501	HCA	C2-C1	5.11	1.66	1.50
4	C	501	HCA	O7-C3	4.92	1.52	1.43
4	C	501	HCA	C2-C3	-4.82	1.47	1.53
4	A	501	HCA	C2-C1	4.48	1.64	1.50
4	A	501	HCA	C3-C7	4.16	1.57	1.53
4	A	501	HCA	O7-C3	4.00	1.51	1.43
4	C	501	HCA	O6-C7	-3.24	1.18	1.30
4	A	501	HCA	O6-C7	-3.00	1.19	1.30
4	C	501	HCA	C3-C7	2.96	1.56	1.53
4	A	501	HCA	O3-C6	2.69	1.31	1.22
4	C	501	HCA	O5-C7	2.47	1.30	1.22
4	A	501	HCA	O5-C7	2.16	1.29	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	501	HCA	O2-C1-O1	7.28	141.45	123.30
4	A	501	HCA	O2-C1-O1	5.70	137.52	123.30
4	A	501	HCA	C4-C5-C6	4.09	122.01	112.75
4	C	501	HCA	O1-C1-C2	-3.99	111.27	122.94
4	C	501	HCA	C4-C5-C6	3.57	120.83	112.75
4	C	501	HCA	O6-C7-C3	3.54	119.20	113.05
4	A	501	HCA	O1-C1-C2	-3.43	112.93	122.94
7	B	2907	EDO	O1-C1-C2	3.27	135.40	111.91
4	A	501	HCA	O6-C7-C3	2.84	117.99	113.05
4	C	501	HCA	O3-C6-C5	-2.79	114.12	123.08
4	C	501	HCA	O7-C3-C7	-2.45	105.43	108.86
7	B	2907	EDO	O2-C2-C1	2.42	129.29	111.91
4	C	501	HCA	O2-C1-C2	-2.20	107.27	114.35

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	2907	EDO	O1-C1-C2-O2
4	A	501	HCA	O1-C1-C2-C3
7	B	2904	EDO	O1-C1-C2-O2
7	D	2908	EDO	O1-C1-C2-O2
7	A	2911	EDO	O1-C1-C2-O2
7	B	2906	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	A	2910	EDO	2	0
7	D	2919	EDO	2	0
7	B	2907	EDO	4	0
4	C	501	HCA	1	0
7	B	2906	EDO	1	0
4	A	501	HCA	1	0
7	B	2904	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

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, 95^{th} 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	0 100 100	8, 15, 26, 36	0
1	C	478/478 (100%)	0.02	1 (0%) 95 94	9, 17, 28, 38	0
2	B	519/519 (100%)	-0.34	1 (0%) 95 94	8, 14, 25, 34	0
2	D	519/519 (100%)	-0.20	2 (0%) 92 92	7, 12, 23, 36	0
All	All	1994/1994 (100%)	-0.22	4 (0%) 95 94	7, 14, 26, 38	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	122	VAL	2.8
2	B	119	ASP	2.6
2	D	4	ILE	2.3
1	C	22	THR	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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, 95^{th} 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	B	2906	4/4	0.73	0.18	37,40,41,42	0
7	EDO	A	2910	4/4	0.82	0.30	29,30,32,33	0
3	MG	B	3003	1/1	0.85	0.12	27,27,27,27	0
3	MG	D	3007	1/1	0.86	0.13	29,29,29,29	0
7	EDO	A	2915	4/4	0.87	0.21	25,31,31,31	0
7	EDO	D	2919	4/4	0.87	0.15	23,29,32,34	0
7	EDO	A	2911	4/4	0.90	0.09	28,28,32,32	0
7	EDO	B	2907	4/4	0.90	0.15	16,21,21,29	0
7	EDO	D	2918	4/4	0.90	0.14	16,25,27,28	0
7	EDO	B	2903	4/4	0.90	0.12	21,22,23,24	0
7	EDO	B	2905	4/4	0.91	0.14	22,24,28,35	0
7	EDO	C	2914	4/4	0.91	0.12	23,23,23,24	0
7	EDO	A	2909	4/4	0.92	0.14	17,18,21,22	0
7	EDO	B	2913	4/4	0.93	0.13	19,20,21,22	0
7	EDO	D	2917	4/4	0.94	0.12	14,17,18,20	0
7	EDO	B	2904	4/4	0.94	0.13	17,18,22,22	0
3	MG	B	3004	1/1	0.94	0.06	24,24,24,24	0
7	EDO	A	2912	4/4	0.95	0.14	28,29,30,35	0
4	HCA	C	501	14/14	0.95	0.09	8,11,12,13	0
3	MG	C	3005	1/1	0.95	0.06	16,16,16,16	0
6	CLF	C	505[A]	15/15	0.96	0.09	8,10,11,13	2
6	CLF	C	505[B]	15/15	0.96	0.09	8,10,11,11	2
7	EDO	D	2916	4/4	0.96	0.07	15,15,15,19	0
5	CFM	C	503	17/17	0.97	0.09	9,11,12,13	0
4	HCA	A	501	14/14	0.97	0.07	8,11,13,13	0
3	MG	A	3001	1/1	0.97	0.09	16,16,16,16	0
7	EDO	D	2908	4/4	0.97	0.12	18,19,22,24	0
8	CL	B	2902	1/1	0.97	0.06	17,17,17,17	0
8	CL	D	2901	1/1	0.97	0.06	14,14,14,14	0
3	MG	B	3002	1/1	0.98	0.07	9,9,9,9	0
6	CLF	A	505[A]	15/15	0.98	0.07	9,12,13,14	2
6	CLF	A	505[B]	15/15	0.98	0.07	9,12,13,15	2
3	MG	D	3006	1/1	0.99	0.08	9,9,9,9	0
5	CFM	A	503	17/17	0.99	0.07	9,10,11,12	0

6.5 Other polymers (i)

There are no such residues in this entry.