



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:45 PM GMT

PDB ID : 1QGU
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.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

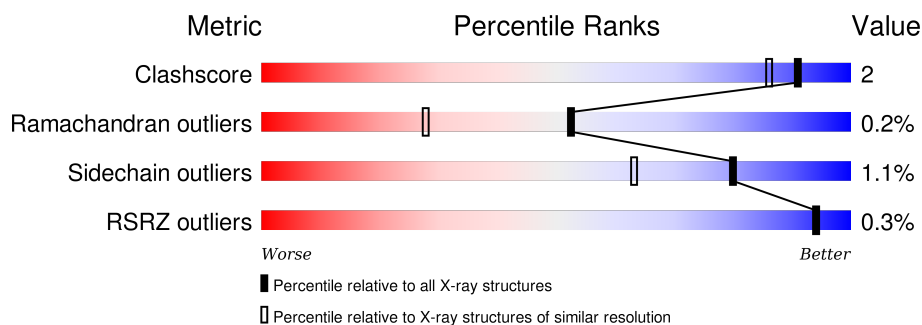
1 Overall quality at a glance

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	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	C	478	
2	B	519	
2	D	519	

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
4	MG	D	3006	-	-	-	X
8	EDO	A	2774	-	-	-	X
8	EDO	A	2775	-	-	-	X
8	EDO	A	2777	-	-	-	X
8	EDO	B	2778	-	-	-	X
8	EDO	B	2781	-	-	-	X
8	EDO	B	2783	-	-	-	X
8	EDO	C	2779	-	-	-	X
8	EDO	D	2773	-	-	-	X
8	EDO	D	2784	-	-	X	X
8	EDO	D	2786	-	-	-	X
8	EDO	D	2788	-	-	-	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			

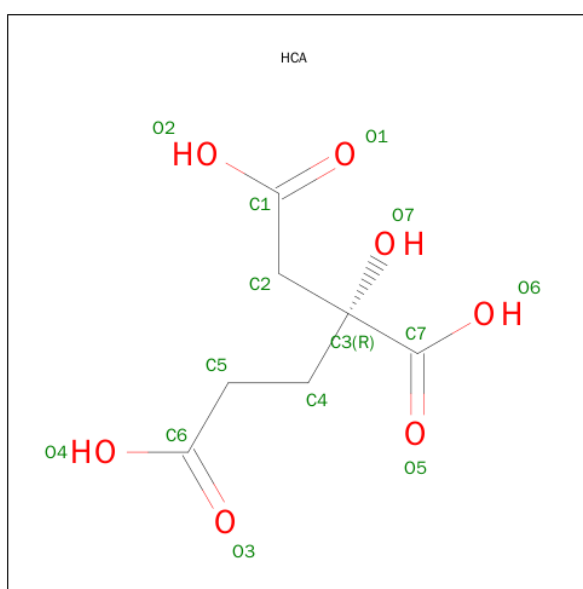
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

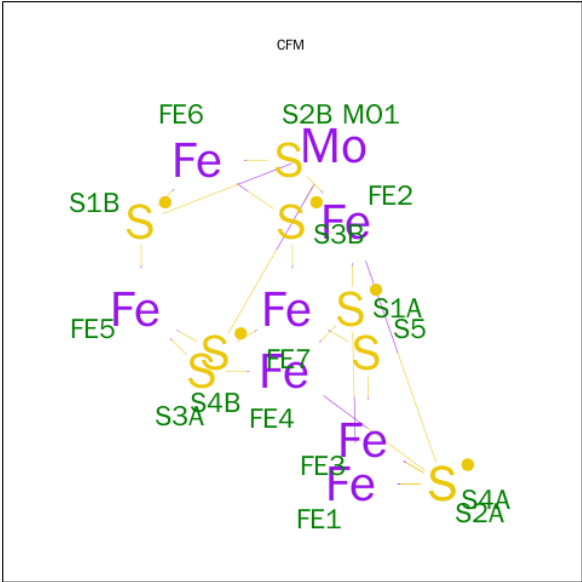
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total Mg 3 3	0	0
4	A	1	Total Mg 1 1	0	0
4	D	2	Total Mg 2 2	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



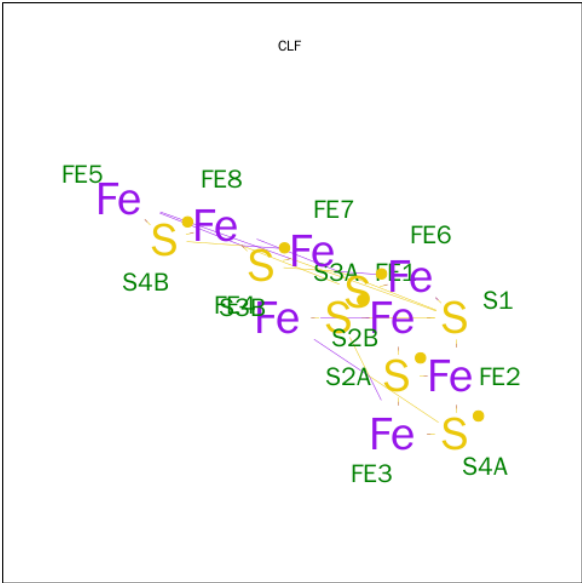
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 14 7 7	0	0
5	C	1	Total C O 14 7 7	0	0

- Molecule 6 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).



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

- Molecule 7 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			15	8	7		
7	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

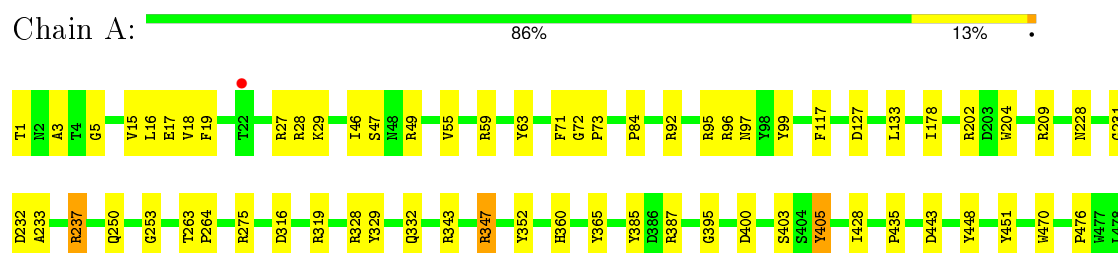
- Molecule 9 is water.

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

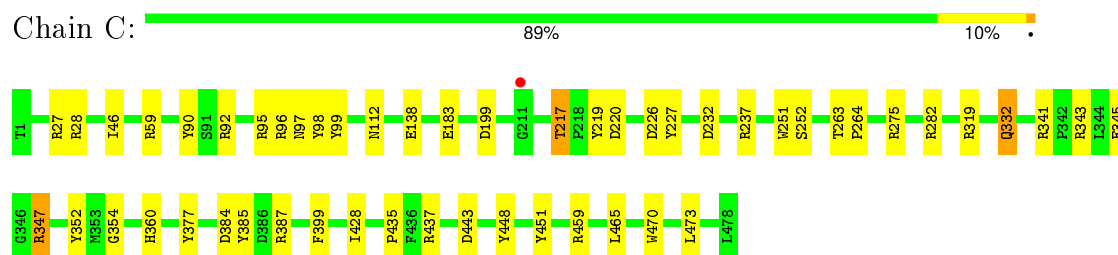
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

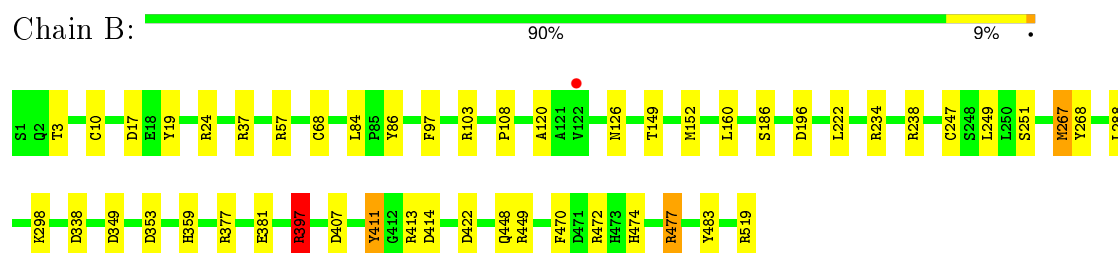
• Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



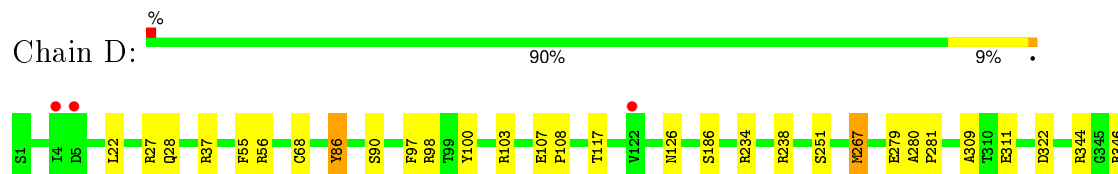
• Molecule 1: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)

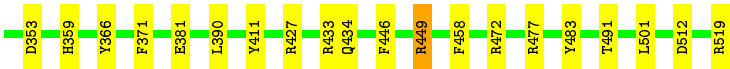


• Molecule 2: PROTEIN (NITROGENASE MOLYBDENUM IRON PROTEIN)



• 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 – 1.60 137.31 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-1.60) 95.4 (137.31-1.60)	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 0.152 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 271680 reflections (0.000%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, CFM, CL, CLF, EDO, HCA

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	0.68	0/3803	1.34	38/5153 (0.7%)
1	C	0.68	0/3813	1.37	42/5165 (0.8%)
2	B	0.71	0/4215	1.49	44/5717 (0.8%)
2	D	0.70	0/4159	1.32	39/5643 (0.7%)
All	All	0.69	0/15990	1.39	163/21678 (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	5
1	C	0	2
2	B	0	2
2	D	0	1
All	All	0	10

There are no bond length outliers.

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	ARG	NE-CZ-NH2	31.31	135.96	120.30
2	B	449	ARG	CD-NE-CZ	19.12	150.37	123.60
2	B	407	ASP	CB-CG-OD2	18.08	134.57	118.30
2	B	103	ARG	NE-CZ-NH1	16.41	128.50	120.30
2	B	397	ARG	NE-CZ-NH1	-16.15	112.23	120.30
2	B	24	ARG	NE-CZ-NH2	-15.45	112.57	120.30
2	D	103	ARG	NE-CZ-NH2	-12.68	113.96	120.30
2	B	24	ARG	NE-CZ-NH1	12.27	126.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	234	ARG	NE-CZ-NH1	10.47	125.53	120.30
2	B	411	TYR	CB-CG-CD1	-10.17	114.90	121.00
2	B	377	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	95	ARG	NE-CZ-NH2	-10.13	115.23	120.30
2	B	519	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	D	519	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	A	237	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	C	347	ARG	NE-CZ-NH2	-9.75	115.42	120.30
2	D	427	ARG	NE-CZ-NH2	-9.60	115.50	120.30
2	B	238	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	C	352	TYR	CB-CG-CD2	9.47	126.68	121.00
2	D	234	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	209	ARG	NE-CZ-NH1	9.43	125.02	120.30
2	B	103	ARG	NE-CZ-NH2	-9.42	115.59	120.30
2	B	519	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	C	347	ARG	NE-CZ-NH1	8.97	124.79	120.30
2	D	103	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	C	96	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	C	28	ARG	CD-NE-CZ	8.85	135.98	123.60
1	A	28	ARG	NE-CZ-NH1	8.65	124.63	120.30
2	B	24	ARG	CD-NE-CZ	8.57	135.60	123.60
2	B	238	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	C	387	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	B	413	ARG	NE-CZ-NH1	8.50	124.55	120.30
2	B	472	ARG	NE-CZ-NH1	8.44	124.52	120.30
2	B	234	ARG	NE-CZ-NH2	-8.44	116.08	120.30
2	D	472	ARG	NE-CZ-NH2	-8.42	116.09	120.30
2	D	322	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	275	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	C	237	ARG	NE-CZ-NH1	8.24	124.42	120.30
2	B	97	PHE	CB-CG-CD2	-8.10	115.13	120.80
2	B	483	TYR	CB-CG-CD2	-8.01	116.20	121.00
1	A	275	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	C	437	ARG	NE-CZ-NH2	-7.75	116.42	120.30
2	B	97	PHE	CB-CG-CD1	7.72	126.21	120.80
2	D	519	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	B	349	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	C	275	ARG	NE-CZ-NH2	-7.63	116.49	120.30
2	B	472	ARG	NE-CZ-NH2	-7.57	116.51	120.30
2	B	353	ASP	CB-CG-OD2	-7.53	111.53	118.30
2	B	349	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	405	TYR	CB-CG-CD1	-7.27	116.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	343	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	400	ASP	CB-CG-OD2	7.13	124.72	118.30
1	C	95	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	C	448	TYR	CB-CG-CD1	7.12	125.27	121.00
1	A	352	TYR	CB-CG-CD2	7.10	125.26	121.00
1	C	341	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	448	TYR	CB-CG-CD2	-6.95	116.83	121.00
2	D	56	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	D	353	ASP	CB-CG-OD1	6.94	124.55	118.30
1	C	98	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	A	319	ARG	NE-CZ-NH2	-6.90	116.85	120.30
2	B	397	ARG	NH1-CZ-NH2	-6.89	111.82	119.40
1	A	63	TYR	CB-CG-CD1	-6.82	116.91	121.00
2	B	407	ASP	OD1-CG-OD2	-6.76	110.46	123.30
1	C	459	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	27	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	448	TYR	CB-CG-CD2	-6.72	116.97	121.00
2	D	446	PHE	CB-CG-CD2	-6.64	116.15	120.80
1	C	451	TYR	CB-CG-CD2	-6.55	117.07	121.00
2	D	238	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	227	TYR	CB-CG-CD2	-6.53	117.08	121.00
2	B	17	ASP	CB-CG-OD1	6.52	124.17	118.30
2	B	196	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	C	437	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	387	ARG	NE-CZ-NH2	-6.41	117.10	120.30
2	D	477	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	405	TYR	CB-CG-CD2	6.36	124.81	121.00
1	A	232	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	C	59	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	385	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	C	385	TYR	CB-CG-CD1	-6.24	117.26	121.00
2	D	107	GLU	OE1-CD-OE2	-6.21	115.85	123.30
2	B	268	TYR	CB-CG-CD2	-6.16	117.30	121.00
2	D	353	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	95	ARG	CG-CD-NE	6.13	124.67	111.80
1	A	316	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	D	433	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	96	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	448	TYR	CB-CG-CD1	6.01	124.61	121.00
2	B	338	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	282	ARG	NE-CZ-NH2	5.99	123.29	120.30
2	D	97	PHE	CB-CG-CD2	-5.98	116.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	371	PHE	CB-CG-CD2	-5.95	116.64	120.80
1	A	343	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	96	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	D	346	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	328	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	28	ARG	CD-NE-CZ	5.91	131.87	123.60
1	C	183	GLU	OE1-CD-OE2	5.90	130.38	123.30
1	C	59	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	90	TYR	CB-CG-CD2	5.89	124.53	121.00
1	A	127	ASP	CB-CG-OD1	5.88	123.59	118.30
2	D	472	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	459	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	384	ASP	CB-CG-OD1	-5.79	113.09	118.30
2	D	512	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	341	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	B	37	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	B	477	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	D	97	PHE	CB-CG-CD1	5.69	124.78	120.80
1	C	352	TYR	CG-CD2-CE2	5.68	125.85	121.30
1	A	27	ARG	NE-CZ-NH1	-5.68	117.46	120.30
2	D	267[A]	MET	CA-CB-CG	5.67	122.95	113.30
2	D	267[B]	MET	CA-CB-CG	5.67	122.95	113.30
1	A	202	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	D	100	TYR	CG-CD1-CE1	-5.65	116.78	121.30
2	B	470	PHE	CB-CG-CD2	-5.62	116.87	120.80
1	C	319	ARG	NE-CZ-NH1	-5.60	117.50	120.30
2	B	422	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	71	PHE	CB-CG-CD2	-5.54	116.92	120.80
2	B	338	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	B	411	TYR	CB-CG-CD2	5.50	124.30	121.00
2	B	57	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	C	332	GLN	CA-CB-CG	5.44	125.38	113.40
1	C	226	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	28	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	451	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	A	47	SER	O-C-N	-5.39	114.07	122.70
2	D	86	TYR	CB-CG-CD2	-5.39	117.77	121.00
2	D	309	ALA	N-CA-CB	5.38	117.64	110.10
2	D	90[A]	SER	N-CA-CB	-5.38	102.43	110.50
2	D	90[B]	SER	N-CA-CB	-5.38	102.43	110.50
2	D	344	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	D	483	TYR	CB-CG-CD2	-5.37	117.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	267[A]	MET	CB-CG-SD	5.37	128.49	112.40
2	D	267[B]	MET	CB-CG-SD	5.37	128.49	112.40
1	A	316	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	92	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	59	ARG	CD-NE-CZ	-5.29	116.19	123.60
1	C	377	TYR	CA-CB-CG	5.28	123.42	113.40
2	D	55	PHE	CB-CG-CD1	-5.25	117.12	120.80
1	C	199	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	329	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	B	247[A]	CYS	CA-CB-SG	5.23	123.41	114.00
2	B	247[B]	CYS	CA-CB-SG	5.23	123.41	114.00
1	A	99	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	C	384	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	37	ARG	CD-NE-CZ	5.21	130.89	123.60
1	C	232	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	365	TYR	CG-CD1-CE1	-5.18	117.15	121.30
2	D	512	ASP	CB-CG-OD1	5.18	122.96	118.30
2	D	37	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	D	27	ARG	NE-CZ-NH2	5.11	122.85	120.30
2	D	98	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	95	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	399	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	A	92	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	D	519	ARG	CG-CD-NE	5.07	122.44	111.80
2	B	86	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	C	138	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	C	282	ARG	CD-NE-CZ	5.05	130.66	123.60
1	A	117	PHE	CB-CG-CD2	-5.04	117.27	120.80
2	B	19	TYR	CB-CG-CD2	5.03	124.02	121.00

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

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Mol	Chain	Res	Type	Group
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	19	0
1	C	3712	0	3576	11	0
2	B	4069	0	3924	16	0
2	D	4047	0	3910	20	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	14	0	6	1	0
5	C	14	0	6	0	0
6	A	17	0	0	0	0
6	C	17	0	0	0	0
7	A	15	0	0	1	0
7	C	15	0	0	0	0
8	A	20	0	30	0	0
8	B	16	0	23	1	0
8	C	4	0	6	0	0
8	D	24	0	36	10	0
9	A	606	0	0	2	0
9	B	794	0	0	6	0
9	C	571	0	0	4	0
9	D	798	0	0	5	0
All	All	18462	0	15081	68	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 (68) 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	8:D:2788:EDO:C1	2.02	0.90
2:D:491:THR:OG1	8:D:2784:EDO:H21	1.75	0.87
2:D:28:GLN:HA	8: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	8:D:2788:EDO:H11	1.74	0.69
2:D:501:LEU:HD21	8:D:2786:EDO:H11	1.74	0.68
2:D:491:THR:HG21	8: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	8:D:2784:EDO:H22	1.79	0.63
8:D:2786:EDO:C1	9:D:3010:HOH:O	2.50	0.60
2:B:84:LEU:HD13	2:B:267[B]:MET:CE	2.33	0.59
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
8: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:HE3	1.89	0.54
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:84:PRO:HB2	7: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
1:A:29:LYS:HB3	1:A:46:ILE:HG12	1.95	0.48
1:C:345:GLU:HG2	9:C:1907:HOH:O	2.15	0.47
1:A:133:LEU:C	1:A:133:LEU:HD23	2.35	0.47
1:A:237:ARG:HD2	1:A:250:GLN:OE1	2.15	0.46
8: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:434:GLN:NE2	2:D:458:PHE:HA	2.32	0.45
9:A:3122:HOH:O	2:D:359:HIS:HB2	2.17	0.45
2:B:68:CYS:HB2	2:B:186:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:C:1882:HOH:O	2:D:117:THR:HG22	2.17	0.43
5:A:501:HCA:O7	5:A:501:HCA:O2	2.36	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:A:263:THR:N	1:A:264:PRO:CD	2.81	0.43
1:C:99:TYR:HE2	9:C:1725:HOH:O	2.02	0.43
1:A:72:GLY:N	1:A:73:PRO:CD	2.82	0.43
1:A:1:THR:OG1	1:A:5:GLY:HA3	2.19	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
2:D:68:CYS:HB2	2:D:186:SER:CB	2.49	0.42
1:C:332:GLN:NE2	9:C:1770:HOH:O	2.53	0.42
1:A:347:ARG:NH2	9:A:3445:HOH:O	2.50	0.41
2:D:366:TYR:HA	2:D:390:LEU:O	2.20	0.41
2:B:149:THR:HG23	2:B:160:LEU:HD11	2.02	0.41
2:B:474:HIS:O	8:D:2784:EDO:H12	2.21	0.41
2:D:449:ARG:HD3	2:D:449:ARG:HH11	1.64	0.41
1:A:16:LEU:HD22	1:A:19:PHE:CE2	2.55	0.41
1:C:263:THR:N	1:C:264:PRO:CD	2.84	0.41
1:A:15:VAL:O	1:A:18:VAL:HG12	2.21	0.40
2:D:22:LEU:HD23	2:D:22:LEU:C	2.41	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

5.3.1 Protein backbone

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%)	39	17
2	D	520/519 (100%)	512 (98%)	7 (1%)	1 (0%)	52	28
All	All	2007/1994 (101%)	1954 (97%)	50 (2%)	3 (0%)	52	31

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 ⓘ

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%)	374 (99%)	4 (1%)	80	63
1	C	379/397 (96%)	373 (98%)	6 (2%)	70	47
2	B	432/442 (98%)	427 (99%)	5 (1%)	78	60
2	D	428/442 (97%)	423 (99%)	5 (1%)	78	60
All	All	1617/1678 (96%)	1597 (99%)	20 (1%)	80	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	347	ARG
1	A	360	HIS
1	A	443	ASP
2	B	126	ASN
2	B	152	MET
2	B	267[A]	MET
2	B	267[B]	MET

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Mol	Chain	Res	Type
2	B	397	ARG
1	C	97	ASN
1	C	112	ASN
1	C	217	THR
1	C	360	HIS
1	C	443	ASP
1	C	473	LEU
2	D	86	TYR
2	D	126	ASN
2	D	267[A]	MET
2	D	267[B]	MET
2	D	449	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	167	ASN
2	B	36	GLN
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

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 carbohydrates 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
8	EDO	A	2774	-	3,3,3	0.43	0	2,2,2	0.52	0
8	EDO	A	2775	-	3,3,3	0.51	0	2,2,2	0.84	0
8	EDO	A	2776	-	3,3,3	0.46	0	2,2,2	0.22	0
8	EDO	A	2777	-	3,3,3	0.56	0	2,2,2	0.61	0
8	EDO	A	2780	-	3,3,3	0.24	0	2,2,2	0.36	0
5	HCA	A	501	-	4,13,13	4.15	2 (50%)	3,18,18	2.63	1 (33%)
6	CFM	A	503	1	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	A	505	1,2	0,24,24	0.00	-	0,57,57	0.00	-
8	EDO	B	2778	-	3,3,3	0.59	0	2,2,2	0.60	0
8	EDO	B	2781	-	3,3,3	0.39	0	2,2,2	0.49	0
8	EDO	B	2782	-	3,3,3	0.07	0	2,2,2	0.54	0
8	EDO	B	2783	-	3,3,3	0.19	0	2,2,2	0.28	0
8	EDO	C	2779	-	3,3,3	0.43	0	2,2,2	0.52	0
5	HCA	C	501	-	4,13,13	3.72	2 (50%)	3,18,18	2.14	1 (33%)
6	CFM	C	503	1	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	C	505	1,2	0,24,24	0.00	-	0,57,57	0.00	-
8	EDO	D	2773	-	3,3,3	0.49	0	2,2,2	0.27	0
8	EDO	D	2784	-	3,3,3	0.76	0	2,2,2	2.73	1 (50%)
8	EDO	D	2785	-	3,3,3	0.66	0	2,2,2	0.09	0
8	EDO	D	2786	-	3,3,3	0.47	0	2,2,2	1.69	1 (50%)
8	EDO	D	2787	-	3,3,3	0.53	0	2,2,2	0.13	0
8	EDO	D	2788	-	3,3,3	0.48	0	2,2,2	0.43	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
8	EDO	A	2774	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2775	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	2776	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2777	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2780	-	-	0/1/1/1	0/0/0/0
5	HCA	A	501	-	-	0/7/17/17	0/0/0/0
6	CFM	A	503	1	-	0/0/84/84	0/0/8/8
7	CLF	A	505	1,2	-	0/0/132/132	0/12/10/10
8	EDO	B	2778	-	-	0/1/1/1	0/0/0/0
8	EDO	B	2781	-	-	0/1/1/1	0/0/0/0
8	EDO	B	2782	-	-	0/1/1/1	0/0/0/0
8	EDO	B	2783	-	-	0/1/1/1	0/0/0/0
8	EDO	C	2779	-	-	0/1/1/1	0/0/0/0
5	HCA	C	501	-	-	0/7/17/17	0/0/0/0
6	CFM	C	503	1	-	0/0/84/84	0/0/8/8
7	CLF	C	505	1,2	-	0/0/132/132	0/12/10/10
8	EDO	D	2773	-	-	0/1/1/1	0/0/0/0
8	EDO	D	2784	-	-	0/1/1/1	0/0/0/0
8	EDO	D	2785	-	-	0/1/1/1	0/0/0/0
8	EDO	D	2786	-	-	0/1/1/1	0/0/0/0
8	EDO	D	2787	-	-	0/1/1/1	0/0/0/0
8	EDO	D	2788	-	-	0/1/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	HCA	C2-C3	-5.24	1.46	1.54
5	C	501	HCA	C2-C3	-4.97	1.47	1.54
5	C	501	HCA	O7-C3	5.35	1.51	1.43
5	A	501	HCA	O7-C3	6.26	1.53	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	2786	EDO	O2-C2-C1	-2.38	95.47	112.54
8	D	2784	EDO	O1-C1-C2	3.30	136.18	112.54
5	C	501	HCA	C4-C3-C2	3.58	123.35	111.33
5	A	501	HCA	C4-C3-C2	4.11	125.12	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	HCA	1	0
7	A	505	CLF	1	0
8	B	2782	EDO	1	0
8	D	2784	EDO	4	0
8	D	2786	EDO	3	0
8	D	2788	EDO	3	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%)	-0.72	1 (0%) 95 94	8, 15, 26, 35	0
1	C	478/478 (100%)	-0.61	1 (0%) 95 94	9, 17, 27, 35	0
2	B	519/519 (100%)	-0.74	1 (0%) 95 94	8, 13, 26, 35	0
2	D	519/519 (100%)	-0.77	3 (0%) 90 90	8, 12, 23, 36	0
All	All	1994/1994 (100%)	-0.71	6 (0%) 94 94	8, 14, 26, 36	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	4	ILE	3.4
2	B	122	VAL	3.0
2	D	5	ASP	2.5
2	D	122	VAL	2.2
1	A	22	THR	2.2
1	C	211	GLY	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
8	EDO	D	2784	4/4	0.94	0.17	24.20	17,20,22,29	0
8	EDO	D	2788	4/4	0.39	0.53	22.13	51,51,52,53	0
8	EDO	D	2786	4/4	0.89	0.19	20.87	16,27,31,31	0
8	EDO	D	2773	4/4	0.92	0.12	13.22	20,20,21,26	0
8	EDO	B	2778	4/4	0.92	0.13	12.10	19,21,21,27	0
8	EDO	A	2775	4/4	0.91	0.19	10.96	30,31,34,35	0
8	EDO	B	2781	4/4	0.94	0.10	6.20	20,21,22,23	0
8	EDO	A	2777	4/4	0.91	0.09	3.06	26,28,28,34	0
8	EDO	A	2774	4/4	0.95	0.09	2.95	17,18,21,22	0
4	MG	D	3006	1/1	0.99	0.07	2.67	10,10,10,10	0
8	EDO	B	2783	4/4	0.97	0.08	2.15	17,25,28,29	0
8	EDO	C	2779	4/4	0.96	0.07	2.11	22,24,25,25	0
5	HCA	C	501	14/14	0.97	0.07	1.42	8,10,14,14	0
8	EDO	D	2785	4/4	0.96	0.07	1.06	15,17,18,20	0
8	EDO	A	2776	4/4	0.88	0.09	0.87	28,29,30,31	0
4	MG	A	3001	1/1	0.98	0.06	0.66	17,17,17,17	0
8	EDO	D	2787	4/4	0.97	0.09	0.54	16,26,30,31	0
5	HCA	A	501	14/14	0.98	0.06	0.50	8,10,13,14	0
6	CFM	A	503	17/17	0.99	0.05	0.15	8,10,10,11	0
4	MG	B	3002	1/1	0.99	0.05	-0.24	9,9,9,9	0
7	CLF	A	505	15/15	0.99	0.05	-0.38	8,11,13,13	0
6	CFM	C	503	17/17	0.99	0.05	-0.94	10,11,12,13	0
7	CLF	C	505	15/15	0.99	0.05	-0.94	7,10,12,12	0
4	MG	C	3005	1/1	0.98	0.04	-1.54	16,16,16,16	0
3	CL	D	2771	1/1	1.00	0.05	-1.84	14,14,14,14	0
3	CL	B	2772	1/1	0.99	0.03	-4.28	16,16,16,16	0
8	EDO	B	2782	4/4	0.94	0.09	-	22,22,26,35	0
8	EDO	A	2780	4/4	0.92	0.17	-	23,30,31,32	0
4	MG	B	3003	1/1	0.98	0.06	-	20,20,20,20	0
4	MG	B	3004	1/1	0.98	0.07	-	19,19,19,19	0
4	MG	D	3007	1/1	0.92	0.08	-	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.