Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:36 pm BST

PDB ID	:	5N78
Title	:	Crystal structure of the cytosolic domain of the CorA Mg2+ channel from Escherichia coli in complex with magnesium and cobalt hexammine
Authors	:	Lerche, M.; Sandhu, H.; Flockner, L.; Hogbom, M.; Rapp, M.
Deposited on	:	2017-02-20
Resolution	:	2.85 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 following versions of software and data (see references ①) were used in the production of this report:

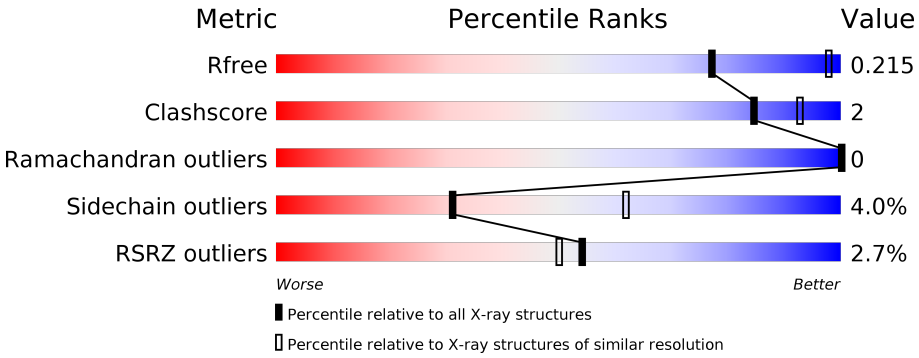
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.85 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))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 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	257	4% 93% 7%
1	B	257	% 89% 9%
1	C	257	88% 11%
1	D	257	5% 95% 5%
1	E	257	3% 92% 8%

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
3	NCO	B	305	-	-	-	X
3	NCO	E	303	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10611 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.

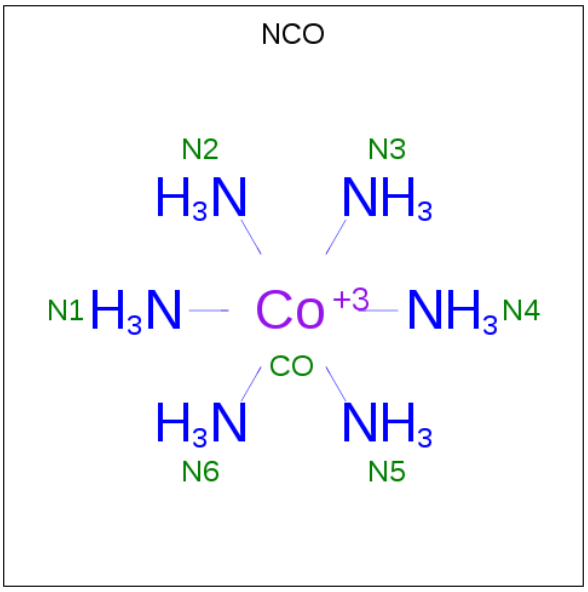
- Molecule 1 is a protein called Magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2081	1308	360	405	8			
1	B	257	Total	C	N	O	S	0	0	0
			2088	1310	362	408	8			
1	C	254	Total	C	N	O	S	0	0	0
			2059	1296	355	400	8			
1	D	257	Total	C	N	O	S	0	0	0
			2076	1304	359	405	8			
1	E	257	Total	C	N	O	S	0	0	0
			2082	1307	359	408	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

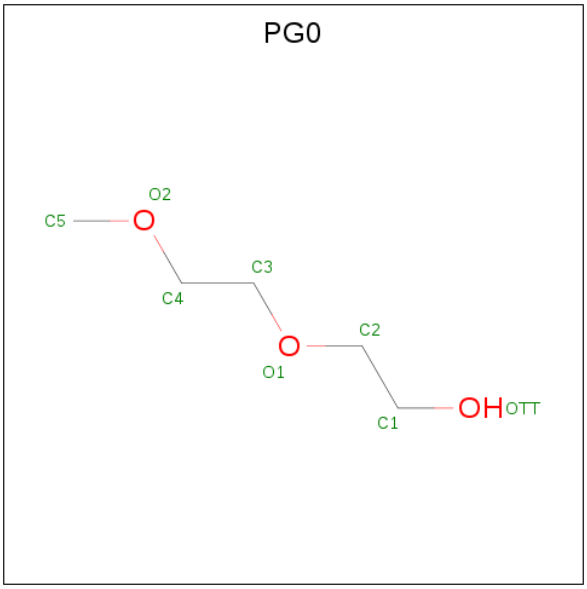
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	2	Total	Mg	0	0
			2	2		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

- Molecule 3 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $CoH_{18}N_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co N 7 1 6	0	0
3	A	1	Total Co N 7 1 6	0	0
3	A	1	Total Co N 7 1 6	0	0
3	B	1	Total Co N 7 1 6	0	0
3	B	1	Total Co N 7 1 6	0	0
3	B	1	Total Co N 7 1 6	0	0
3	C	1	Total Co N 7 1 6	0	0
3	C	1	Total Co N 7 1 6	0	0
3	D	1	Total Co N 7 1 6	0	0
3	D	1	Total Co N 7 1 6	0	0
3	D	1	Total Co N 7 1 6	0	0
3	E	1	Total Co N 7 1 6	0	0
3	E	1	Total Co N 7 1 6	0	0
3	E	1	Total Co N 7 1 6	0	0

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 8 5 3	0	0
4	C	1	Total C O 8 5 3	0	0
4	E	1	Total C O 8 5 3	0	0

- Molecule 5 is water.

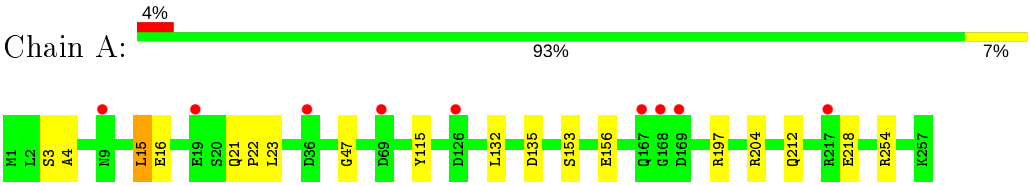
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	15	Total O 15 15	0	0
5	B	23	Total O 23 23	0	0
5	C	23	Total O 23 23	0	0
5	D	18	Total O 18 18	0	0
5	E	18	Total O 18 18	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

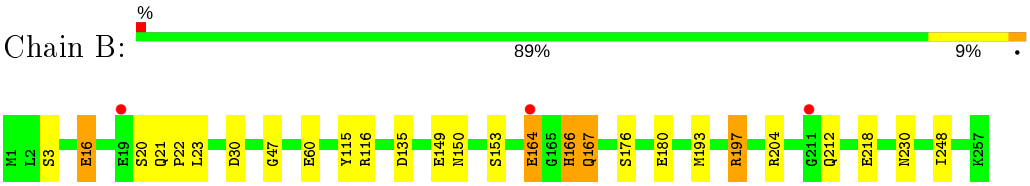
- Molecule 1: Magnesium transport protein CorA

Chain A:



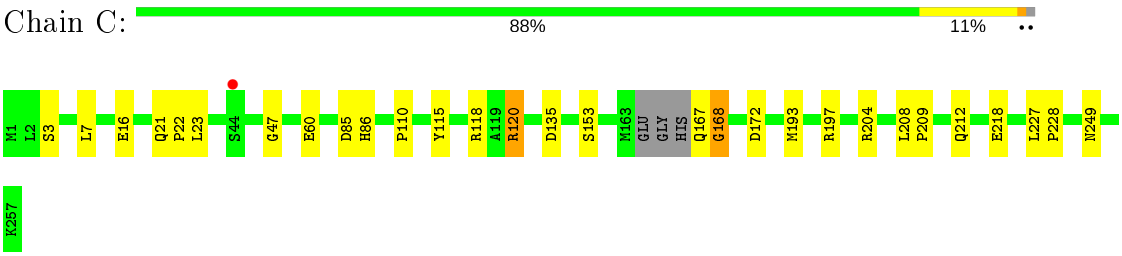
- Molecule 1: Magnesium transport protein CorA

Chain B:



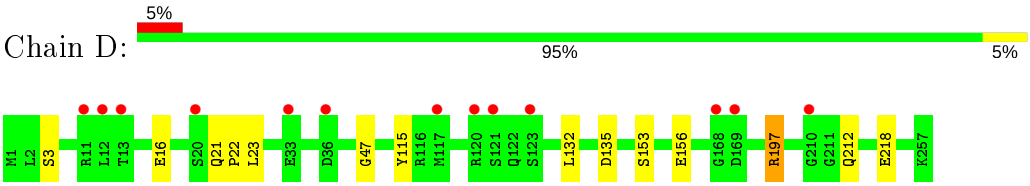
- Molecule 1: Magnesium transport protein CorA

Chain C:



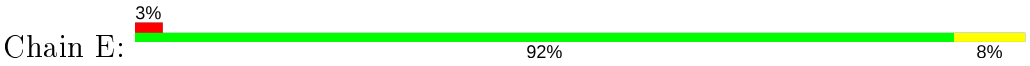
- Molecule 1: Magnesium transport protein CorA

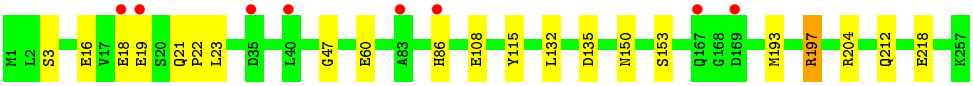
Chain D:



- Molecule 1: Magnesium transport protein CorA

Chain E:




M1
L2
S3
E16
V17
E18
E19
S20
Q21
P22
L23
D35
L40
G47
E60
A83
H86
E108
Y115
L132
D135
N150
S153
Q167
G168
D169
M193
R197
R204
Q212
E218
K257

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.72Å 117.32Å 91.86Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	29.44 – 2.85 29.44 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.44-2.85) 98.3 (29.44-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.178 , 0.218 0.182 , 0.215	Depositor DCC
R_{free} test set	1769 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.2	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	10611	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PG0, NCO

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	0.59	0/2114	0.74	1/2853 (0.0%)
1	B	0.65	0/2120	0.77	1/2860 (0.0%)
1	C	0.63	0/2090	0.75	2/2819 (0.1%)
1	D	0.57	0/2108	0.71	0/2845
1	E	0.61	0/2114	0.76	1/2853 (0.0%)
All	All	0.61	0/10546	0.75	5/14230 (0.0%)

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	1
1	B	0	3
1	C	0	2
1	D	0	1
1	E	0	1
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	GLN	N-CA-C	6.90	129.64	111.00
1	A	204	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	E	204	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	120	ARG	N-CA-C	-5.70	95.61	111.00
1	C	204	ARG	CB-CG-CD	5.68	126.38	111.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	GLY	Peptide
1	B	164	GLU	Peptide
1	B	166	HIS	Peptide
1	B	47	GLY	Peptide
1	C	168	GLY	Peptide
1	C	47	GLY	Peptide
1	D	47	GLY	Peptide
1	E	47	GLY	Peptide

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	2081	0	2019	8	0
1	B	2088	0	2031	16	0
1	C	2059	0	2004	15	0
1	D	2076	0	2017	4	0
1	E	2082	0	2020	8	1
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	21	0	0	0	1
3	B	21	0	0	2	0
3	C	14	0	0	1	0
3	D	21	0	0	0	0
3	E	21	0	0	1	0
4	B	8	0	12	1	0
4	C	8	0	12	0	0
4	E	8	0	12	2	0
5	A	15	0	0	0	0
5	B	23	0	0	4	0
5	C	23	0	0	6	0
5	D	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	18	0	0	2	0
All	All	10611	0	10127	48	1

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 (48) 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)
1:C:85:ASP:OD1	3:C:304:NCO:N1	2.00	0.93
1:B:149:GLU:OE1	3:B:305:NCO:N4	2.04	0.91
1:C:209:PRO:HD3	5:C:406:HOH:O	1.75	0.85
1:B:30:ASP:OD2	5:B:401:HOH:O	2.03	0.76
1:C:118:ARG:O	1:C:120:ARG:O	2.04	0.76
1:B:116:ARG:HD2	5:B:401:HOH:O	1.86	0.74
1:E:150:ASN:OD1	3:E:304:NCO:N4	2.27	0.68
1:B:16:GLU:CD	1:B:16:GLU:H	1.97	0.67
1:B:16:GLU:HG2	1:B:20:SER:HB3	1.75	0.67
1:E:108:GLU:OE1	5:E:401:HOH:O	2.14	0.64
1:C:193:MET:HE2	5:C:419:HOH:O	1.96	0.64
1:C:209:PRO:CD	5:C:406:HOH:O	2.42	0.61
1:A:4:ALA:O	1:A:15:LEU:HD13	2.01	0.60
1:E:115:TYR:CE1	5:E:407:HOH:O	2.52	0.59
1:D:197:ARG:HD2	5:D:408:HOH:O	2.02	0.59
1:B:167:GLN:NE2	1:B:248:ILE:HA	2.18	0.57
1:B:150:ASN:ND2	3:B:305:NCO:N2	2.53	0.57
1:D:156:GLU:OE2	1:E:86:HIS:HE1	1.88	0.56
1:B:197:ARG:HD2	5:B:409:HOH:O	2.06	0.54
1:B:115:TYR:CE1	1:B:135:ASP:HB3	2.43	0.53
1:A:156:GLU:OE2	1:C:86:HIS:HE1	1.92	0.53
1:C:115:TYR:CE1	1:C:135:ASP:HB3	2.43	0.52
1:E:115:TYR:CE1	1:E:135:ASP:HB3	2.45	0.52
1:D:115:TYR:CE1	1:D:135:ASP:HB3	2.45	0.52
1:B:176:SER:O	1:B:180:GLU:HG2	2.10	0.52
1:B:164:GLU:O	1:B:166:HIS:CB	2.58	0.52
1:E:197:ARG:HD2	4:E:302:PG0:C5	2.41	0.51
1:A:115:TYR:CE1	1:A:135:ASP:HB3	2.45	0.50
1:B:204:ARG:HH11	1:B:204:ARG:HA	1.78	0.49
1:A:21:GLN:N	1:A:22:PRO:HD2	2.28	0.48
1:D:21:GLN:N	1:D:22:PRO:HD2	2.29	0.48
1:C:208:LEU:HA	5:C:406:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLN:N	1:B:22:PRO:HD2	2.29	0.47
1:A:4:ALA:C	1:A:15:LEU:HD13	2.33	0.47
1:C:21:GLN:N	1:C:22:PRO:HD2	2.29	0.47
1:B:167:GLN:HE22	1:B:248:ILE:HA	1.79	0.47
1:A:254:ARG:NH2	1:C:172:ASP:OD2	2.49	0.46
1:C:7:LEU:HD23	5:C:421:HOH:O	2.15	0.45
1:E:21:GLN:N	1:E:22:PRO:HD2	2.31	0.45
1:A:4:ALA:C	1:A:15:LEU:CD1	2.86	0.44
1:C:167:GLN:N	1:C:168:GLY:CA	2.81	0.43
5:B:403:HOH:O	1:C:249:ASN:CG	2.56	0.43
1:C:110:PRO:HD2	5:C:414:HOH:O	2.19	0.43
1:E:193:MET:HG3	4:E:302:PG0:H22	2.01	0.43
1:A:21:GLN:N	1:A:22:PRO:CD	2.83	0.42
1:C:227:LEU:N	1:C:228:PRO:CD	2.84	0.41
1:B:193:MET:HG3	4:B:302:PG0:O1	2.22	0.40
1:B:21:GLN:N	1:B:22:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:GLU:OE1	3:A:304:NCO:N4[1_556]	1.96	0.24

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	255/257 (99%)	245 (96%)	10 (4%)	0	100	100
1	B	255/257 (99%)	245 (96%)	10 (4%)	0	100	100
1	C	250/257 (97%)	242 (97%)	8 (3%)	0	100	100
1	D	255/257 (99%)	247 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	255/257 (99%)	247 (97%)	8 (3%)	0	100	100
All	All	1270/1285 (99%)	1226 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	222/227 (98%)	213 (96%)	9 (4%)	30	61
1	B	224/227 (99%)	215 (96%)	9 (4%)	31	62
1	C	220/227 (97%)	212 (96%)	8 (4%)	35	66
1	D	222/227 (98%)	214 (96%)	8 (4%)	35	66
1	E	223/227 (98%)	213 (96%)	10 (4%)	27	57
All	All	1111/1135 (98%)	1067 (96%)	44 (4%)	31	62

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	15	LEU
1	A	16	GLU
1	A	23	LEU
1	A	132	LEU
1	A	153	SER
1	A	197	ARG
1	A	212	GLN
1	A	218	GLU
1	B	3	SER
1	B	16	GLU
1	B	23	LEU
1	B	60	GLU
1	B	153	SER

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Mol	Chain	Res	Type
1	B	197	ARG
1	B	212	GLN
1	B	218	GLU
1	B	230	ASN
1	C	3	SER
1	C	16	GLU
1	C	23	LEU
1	C	60	GLU
1	C	153	SER
1	C	197	ARG
1	C	212	GLN
1	C	218	GLU
1	D	3	SER
1	D	16	GLU
1	D	23	LEU
1	D	132	LEU
1	D	153	SER
1	D	197	ARG
1	D	212	GLN
1	D	218	GLU
1	E	3	SER
1	E	16	GLU
1	E	18	GLU
1	E	23	LEU
1	E	60	GLU
1	E	132	LEU
1	E	153	SER
1	E	197	ARG
1	E	212	GLN
1	E	218	GLU

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	249	ASN
1	B	86	HIS
1	B	150	ASN
1	B	167	GLN
1	B	249	ASN
1	C	86	HIS
1	C	249	ASN
1	D	249	ASN

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Mol	Chain	Res	Type
1	E	86	HIS
1	E	249	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
3	NCO	A	305	-	6,6,6	0.65	0	-		
3	NCO	E	305	-	6,6,6	0.67	0	-		
3	NCO	D	302	-	6,6,6	0.76	0	-		
3	NCO	A	304	-	6,6,6	0.64	0	-		
3	NCO	D	304	-	6,6,6	0.72	0	-		
3	NCO	E	304	-	6,6,6	0.67	0	-		
3	NCO	A	303	-	6,6,6	0.79	0	-		
3	NCO	B	305	-	6,6,6	0.66	0	-		
3	NCO	E	303	-	6,6,6	0.66	0	-		
4	PG0	C	302	-	7,7,7	0.63	0	6,6,6	0.41	0
3	NCO	B	303	-	6,6,6	0.73	0	-		
3	NCO	C	303	-	6,6,6	0.70	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NCO	C	304	-	6,6,6	0.64	0	-		
3	NCO	B	304	-	6,6,6	0.70	0	-		
4	PG0	E	302	-	7,7,7	0.64	0	6,6,6	0.47	0
3	NCO	D	303	-	6,6,6	0.70	0	-		
4	PG0	B	302	-	7,7,7	0.80	0	6,6,6	0.78	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	PG0	C	302	-	-	0/5/5/5	-
4	PG0	E	302	-	-	3/5/5/5	-
4	PG0	B	302	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	PG0	OTT-C1-C2-O1
4	E	302	PG0	OTT-C1-C2-O1
4	B	302	PG0	C3-C4-O2-C5
4	E	302	PG0	C4-C3-O1-C2
4	E	302	PG0	O1-C3-C4-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	NCO	0	1
3	E	304	NCO	1	0
3	B	305	NCO	2	0
3	C	304	NCO	1	0
4	E	302	PG0	2	0
4	B	302	PG0	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	257/257 (100%)	-0.18	9 (3%) 44 38	42, 74, 122, 187	0
1	B	257/257 (100%)	-0.28	3 (1%) 79 78	37, 65, 117, 161	0
1	C	254/257 (98%)	-0.30	1 (0%) 92 92	40, 70, 111, 171	0
1	D	257/257 (100%)	0.01	13 (5%) 28 23	49, 81, 140, 190	0
1	E	257/257 (100%)	-0.16	8 (3%) 49 44	44, 71, 120, 183	0
All	All	1282/1285 (99%)	-0.18	34 (2%) 54 50	37, 72, 126, 190	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	ASP	5.3
1	D	169	ASP	4.5
1	E	19	GLU	4.4
1	E	167	GLN	4.2
1	D	168	GLY	3.3
1	D	36	ASP	3.3
1	B	164	GLU	3.2
1	E	35	ASP	2.9
1	A	36	ASP	2.6
1	D	13	THR	2.6
1	D	11	ARG	2.5
1	A	19	GLU	2.5
1	A	69	ASP	2.5
1	A	167	GLN	2.4
1	A	126	ASP	2.4
1	E	18	GLU	2.4
1	B	211	GLY	2.3
1	E	40	LEU	2.3
1	A	168	GLY	2.3
1	B	19	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	123	SER	2.3
1	E	83	ALA	2.2
1	D	121	SER	2.2
1	D	120	ARG	2.2
1	D	20	SER	2.2
1	E	169	ASP	2.2
1	A	9	ASN	2.2
1	D	210	GLY	2.2
1	E	86	HIS	2.1
1	D	33	GLU	2.1
1	A	217	ARG	2.1
1	D	117	MET	2.1
1	C	44	SER	2.0
1	D	12	LEU	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 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. 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
3	NCO	E	303	7/7	0.56	0.48	172,181,191,196	0
3	NCO	B	305	7/7	0.72	0.43	149,158,164,166	0
4	PG0	E	302	8/8	0.77	0.32	90,104,108,109	0
3	NCO	D	303	7/7	0.81	0.35	152,156,159,163	0
4	PG0	C	302	8/8	0.81	0.29	88,98,107,108	0
3	NCO	C	304	7/7	0.82	0.31	163,167,172,175	0
3	NCO	E	305	7/7	0.82	0.40	169,173,177,180	0
3	NCO	C	303	7/7	0.83	0.35	149,154,165,165	0
3	NCO	A	305	7/7	0.83	0.32	134,144,148,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NCO	B	304	7/7	0.85	0.37	145,153,161,164	0
4	PG0	B	302	8/8	0.85	0.30	82,104,113,116	0
3	NCO	A	304	7/7	0.86	0.36	127,147,149,155	0
3	NCO	D	304	7/7	0.87	0.32	142,152,155,166	0
3	NCO	A	303	7/7	0.89	0.29	106,112,120,122	0
3	NCO	E	304	7/7	0.90	0.25	138,142,151,158	0
3	NCO	D	302	7/7	0.90	0.27	120,131,140,144	0
2	MG	B	301	1/1	0.96	0.20	58,58,58,58	0
2	MG	A	302	1/1	0.96	0.90	69,69,69,69	0
3	NCO	B	303	7/7	0.98	0.17	81,88,90,91	0
2	MG	A	301	1/1	0.98	0.26	50,50,50,50	0
2	MG	D	301	1/1	0.99	0.22	78,78,78,78	0
2	MG	C	301	1/1	0.99	0.15	54,54,54,54	0
2	MG	E	301	1/1	0.99	0.21	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.