wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 11:26 AM EDT

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PDB ID	:	1XE3
Title	:	Crystal Structure of purine nucleoside phosphorylase DeoD from Bacillus anthracis
Authors	:	Grenha, R.; Levdikov, V.M.; Fogg, M.; Blagova, E.V.; Brannigan, J.A.; Wilkinson, A.J.; Wilson, K.S.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2004-09-09
Resolution	:	2.24 Å(reported)

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 2.24 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.
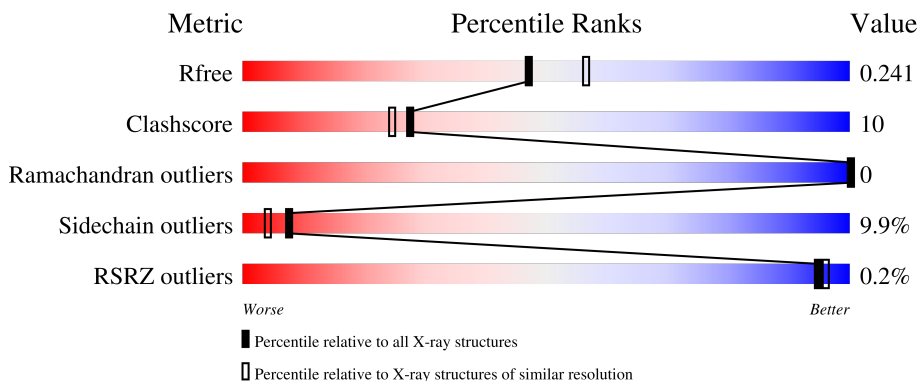
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	245	73% 18% • 5%
1	B	245	76% 13% 6% 5%
1	C	245	77% 14% 5% •
1	D	245	72% 18% 6% •
1	E	245	% 75% 16% • •

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Mol	Chain	Length	Quality of chain
1	F	245	77% 13% 5% 5%

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
2	CL	C	806	-	-	X	-

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11450 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 purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1782	1127	296	347	12			
1	B	233	Total	C	N	O	S	0	0	0
			1780	1127	294	347	12			
1	C	234	Total	C	N	O	S	0	0	0
			1790	1133	297	348	12			
1	D	235	Total	C	N	O	S	0	0	0
			1799	1138	299	350	12			
1	E	234	Total	C	N	O	S	0	0	0
			1789	1132	296	349	12			
1	F	233	Total	C	N	O	S	0	1	0
			1788	1132	297	347	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	cloning artifact	UNP Q81T09
A	-8	GLY	-	cloning artifact	UNP Q81T09
A	-7	SER	-	cloning artifact	UNP Q81T09
A	-6	SER	-	cloning artifact	UNP Q81T09
A	-5	HIS	-	expression tag	UNP Q81T09
A	-4	HIS	-	expression tag	UNP Q81T09
A	-3	HIS	-	expression tag	UNP Q81T09
A	-2	HIS	-	expression tag	UNP Q81T09
A	-1	HIS	-	expression tag	UNP Q81T09
A	0	HIS	-	expression tag	UNP Q81T09
B	-9	MET	-	cloning artifact	UNP Q81T09
B	-8	GLY	-	cloning artifact	UNP Q81T09
B	-7	SER	-	cloning artifact	UNP Q81T09
B	-6	SER	-	cloning artifact	UNP Q81T09
B	-5	HIS	-	expression tag	UNP Q81T09
B	-4	HIS	-	expression tag	UNP Q81T09
B	-3	HIS	-	expression tag	UNP Q81T09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q81T09
B	-1	HIS	-	expression tag	UNP Q81T09
B	0	HIS	-	expression tag	UNP Q81T09
C	-9	MET	-	cloning artifact	UNP Q81T09
C	-8	GLY	-	cloning artifact	UNP Q81T09
C	-7	SER	-	cloning artifact	UNP Q81T09
C	-6	SER	-	cloning artifact	UNP Q81T09
C	-5	HIS	-	expression tag	UNP Q81T09
C	-4	HIS	-	expression tag	UNP Q81T09
C	-3	HIS	-	expression tag	UNP Q81T09
C	-2	HIS	-	expression tag	UNP Q81T09
C	-1	HIS	-	expression tag	UNP Q81T09
C	0	HIS	-	expression tag	UNP Q81T09
D	-9	MET	-	cloning artifact	UNP Q81T09
D	-8	GLY	-	cloning artifact	UNP Q81T09
D	-7	SER	-	cloning artifact	UNP Q81T09
D	-6	SER	-	cloning artifact	UNP Q81T09
D	-5	HIS	-	expression tag	UNP Q81T09
D	-4	HIS	-	expression tag	UNP Q81T09
D	-3	HIS	-	expression tag	UNP Q81T09
D	-2	HIS	-	expression tag	UNP Q81T09
D	-1	HIS	-	expression tag	UNP Q81T09
D	0	HIS	-	expression tag	UNP Q81T09
E	-9	MET	-	cloning artifact	UNP Q81T09
E	-8	GLY	-	cloning artifact	UNP Q81T09
E	-7	SER	-	cloning artifact	UNP Q81T09
E	-6	SER	-	cloning artifact	UNP Q81T09
E	-5	HIS	-	expression tag	UNP Q81T09
E	-4	HIS	-	expression tag	UNP Q81T09
E	-3	HIS	-	expression tag	UNP Q81T09
E	-2	HIS	-	expression tag	UNP Q81T09
E	-1	HIS	-	expression tag	UNP Q81T09
E	0	HIS	-	expression tag	UNP Q81T09
F	-9	MET	-	cloning artifact	UNP Q81T09
F	-8	GLY	-	cloning artifact	UNP Q81T09
F	-7	SER	-	cloning artifact	UNP Q81T09
F	-6	SER	-	cloning artifact	UNP Q81T09
F	-5	HIS	-	expression tag	UNP Q81T09
F	-4	HIS	-	expression tag	UNP Q81T09
F	-3	HIS	-	expression tag	UNP Q81T09
F	-2	HIS	-	expression tag	UNP Q81T09
F	-1	HIS	-	expression tag	UNP Q81T09

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP Q81T09

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	B	1	Total 1	Cl 1	0	0
2	C	2	Total 2	Cl 2	0	0
2	D	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total 148	O 148	0	0
3	B	114	Total 114	O 114	0	0
3	C	115	Total 115	O 115	0	0
3	D	115	Total 115	O 115	0	0
3	E	122	Total 122	O 122	0	0
3	F	102	Total 102	O 102	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.
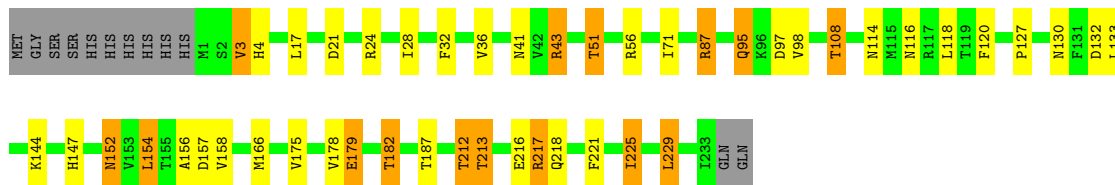
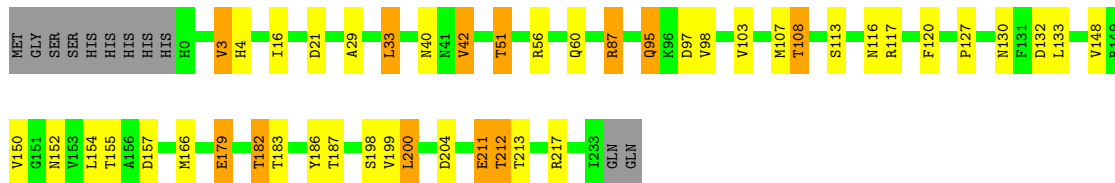- Molecule 1: purine nucleoside phosphorylase

Chain A:
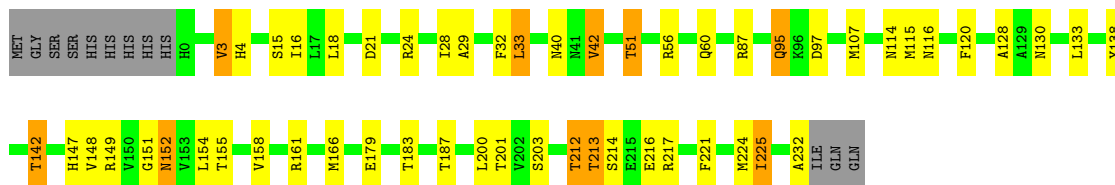
- Molecule 1: purine nucleoside phosphorylase

Chain B:

- Molecule 1: purine nucleoside phosphorylase

Chain C:

- Molecule 1: purine nucleoside phosphorylase

Chain D:

P127 N130 F131 D132 L133 Y138 T142 G151 N152 V153 L154 V158 M166 V167 K168 K169 L170 V175 V178 E179 T182 T183 T187 V199 L200 T212 T213 S214 E215 E216 R217 E226 A232 I233 Q234 GLN

• Molecule 1: purine nucleoside phosphorylase

Chain E:

%

75%   16%   •   •

MET GLY SER SER HIS HIS HIS HIS HIS M1 S2 V3 H4 I16 L17 A29 L33 N40 N41 V42 R43 Q60 M64 Y72 L76 Q95 K96 D97 V98 D102 V103 T108 D112 S113 N114 M115 N116 R117 F120 P127 N130 L133 L134

K135 K136 A137 Y138 T142 H147 N152 V153 L154 T155 E162 M166 V167 E179 T182 T183 T187 S198 T201 T213 E216 R217 M224 I225 L229 Q234 GLN

• Molecule 1: purine nucleoside phosphorylase

Chain F:

77%   13%   5%   5%

MET GLY SER SER HIS HIS HIS HIS HIS M1 S2 V3 H4 A29 L33 E34 D35 V36 N40 N41 V42 R43 R87 Q95 K96 D97 V98 K99 V100 R101 M107 T108 A109 C110 T111 N116 R117 L118 P127 N130 L133 H147 V148 R149 N152 V153 L154

T155 V158 M164 D165 M166 V167 E179 T182 T183 T187 L200 T212 T213 S214 E215 E216 R217 Q218 T219 E226 I233 GLN GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.86Å 128.26Å 223.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.24 19.98 – 2.24	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.24) 90.9 (19.98-2.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.23Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.235 0.188 , 0.241	Depositor DCC
R_{free} test set	4066 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11450	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CL

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	0.63	0/1809	0.79	1/2447 (0.0%)
1	B	0.64	0/1806	0.77	2/2443 (0.1%)
1	C	0.63	0/1817	0.74	0/2458
1	D	0.67	0/1826	0.81	1/2470 (0.0%)
1	E	0.62	0/1815	0.78	1/2455 (0.0%)
1	F	0.64	0/1817	0.75	0/2457
All	All	0.64	0/10890	0.78	5/14730 (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	D	0	1

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	43	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	149	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	E	217	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	24	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	217	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	40	ASN	Peptide

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	1782	0	1787	36	0
1	B	1780	0	1791	41	0
1	C	1790	0	1798	40	0
1	D	1799	0	1806	47	0
1	E	1789	0	1799	36	0
1	F	1788	0	1804	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	2	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
3	A	148	0	0	3	0
3	B	114	0	0	5	0
3	C	115	0	0	3	0
3	D	115	0	0	5	0
3	E	122	0	0	3	0
3	F	102	0	0	3	0
All	All	11450	0	10785	216	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 10.

The worst 5 of 216 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:B:51:THR:HG22	1:B:56:ARG:HH11	1.41	0.85
1:A:158:VAL:HB	3:A:931:HOH:O	1.76	0.84
1:A:138:TYR:O	1:A:142:THR:HG23	1.77	0.84
1:E:138:TYR:O	1:E:142:THR:HG22	1.80	0.81
1:C:120:PHE:HA	1:E:166:MET:HE2	1.64	0.79

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	231/245 (94%)	231 (100%)	0	0	100	100
1	B	231/245 (94%)	228 (99%)	3 (1%)	0	100	100
1	C	232/245 (95%)	229 (99%)	3 (1%)	0	100	100
1	D	233/245 (95%)	231 (99%)	2 (1%)	0	100	100
1	E	232/245 (95%)	227 (98%)	5 (2%)	0	100	100
1	F	232/245 (95%)	230 (99%)	2 (1%)	0	100	100
All	All	1391/1470 (95%)	1376 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	192/203 (95%)	175 (91%)	17 (9%)	9	6
1	B	192/203 (95%)	171 (89%)	21 (11%)	6	3
1	C	193/203 (95%)	175 (91%)	18 (9%)	9	5
1	D	194/203 (96%)	174 (90%)	20 (10%)	7	4
1	E	193/203 (95%)	176 (91%)	17 (9%)	10	6
1	F	193/203 (95%)	170 (88%)	23 (12%)	5	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1157/1218 (95%)	1041 (90%)	116 (10%)	8 4

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	36	VAL
1	F	200	LEU
1	D	170	LEU
1	F	183	THR
1	F	95	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	147	HIS
1	F	147	HIS
1	E	152	ASN
1	F	95	GLN
1	F	195	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 monosaccharides in this entry.

5.6   Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	233/245 (95%)	-0.55	0	100	100	15, 21, 29, 35	0
1	B	233/245 (95%)	-0.54	0	100	100	16, 21, 29, 35	0
1	C	234/245 (95%)	-0.52	0	100	100	14, 21, 28, 35	0
1	D	235/245 (95%)	-0.49	0	100	100	13, 21, 31, 40	0
1	E	234/245 (95%)	-0.41	2 (0%)	84	84	15, 22, 32, 42	0
1	F	233/245 (95%)	-0.44	1 (0%)	92	93	16, 22, 33, 40	0
All	All	1402/1470 (95%)	-0.49	3 (0%)	95	96	13, 21, 31, 42	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	3.5
1	E	162	GLU	2.8
1	F	35	ASP	2.2

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, 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
2	CL	A	805	1/1	0.98	0.06	26,26,26,26	0
2	CL	B	801	1/1	0.99	0.07	23,23,23,23	0
2	CL	C	802	1/1	0.99	0.06	17,17,17,17	0
2	CL	C	806	1/1	0.99	0.22	24,24,24,24	0
2	CL	D	804	1/1	1.00	0.09	16,16,16,16	0
2	CL	F	803	1/1	1.00	0.09	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.